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Planning Report

Economic Impact of Standard Reference Materials for Sulfur in Fossil Fuels

Prepared by:
Research Triangle Institute

for

National Institute of
Standards & Technology

Program Office
Strategic Planning and
Economic Analysis Group

February 2000

U.S Department of Commerce
Technology Administration

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National Institute of Standards and Technology
Bldg. 101, Room A1013
Gaithersburg, MD 20899-1060

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RTI Project Number 7007-006

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Acknowledgments

We wish to acknowledge Dr. Gregory C. Tassey, Dr. W. Robert Kelly, Bruce S. MacDonald, Dr. John D. Fassett, and Ellyn S. Beary for helpful comments and suggestions on earlier versions of this report.

Contents

4. Valuing Improved Sulfur Information 4-1

Appendixes

Figures

Tables

Executive Summary

The National Institute of Standards and Technology (NIST) promotes U.S. economic growth by working with industry to develop and apply technology, measurements, and standards. Through its Office of Standard Reference Materials, NIST is authorized to certify and sell standard reference materials (SRMs) that help users engaged in commerce or research link their measurements to NIST. Developed by NIST's Technical Laboratories, SRMs are materials certified for their chemical composition or physical properties. As emerging regulations increase the importance of the sulfur content of fossil fuels, NIST is expanding its SRM program to include SRMs for measuring sulfur in the low-sulfur fuels required to meet these regulations. The development of an SRM employs NIST's unique expertise in measurement. A NIST-certified SRM carries with it the full weight and authority of NIST and the U.S. Department of Commerce. This study estimates the economic impact of NIST SRMs for sulfur in fossil fuels.

SRMs play a key role in the National Measurement System for Analytical Chemistry. They serve as national primary chemical standards and are used as calibrants and as quality assurance materials to evaluate measurement accuracy, to intercalibrate laboratories in a measurement program, and to provide compatibility of measurement data (Taylor, 1993). The absence of SRMs as primary chemical standards would weaken the entire measurement system.

SRMs help users verify the accuracy of measurement methods or calibrate measurement systems. NIST SRMs greatly improve measurement accuracy by reducing the uncertainty of measurement. These improvements enhance the products and services of the measurement industry, such as testing laboratories and analytical equipment manufacturers. More accurate sulfur content information also reduces the likelihood of disputes between sellers and purchasers of fossil fuels, such as coal companies and electric utilities. Other benefits include better production efficiency for the petroleum industry and lower sulfur emissions to the environment.

This study quantifies a portion of the economic benefits associated with sulfur SRMs. Included in the measures of economic benefits are improvements in product quality, production efficiency, and reductions in transaction costs and sulfur dioxide emissions to the environment. In addition, the study identifies and qualitatively describes the impact of NIST SRMs on other less tangible areas, such as research and development programs.

Table ES-1 presents several measures of economic benefit from NIST's investment in sulfur SRMs based on the impacts quantified as part of this study. Benefit estimates are based on information gathered from industry, and NIST expenditures were provided by NIST's Technical Laboratories. The net present value (NPV) of the economic benefits beginning in 1984 is $409 million ($1998).

Table ES-1. Measures of Economic Benefits from NIST SRMs
Economic impacts reflect benefits and costs beginning in 1984, projected through 2003.

Measure	Economic Impact
Benefit-cost ratio	113
Social rate of return	1,056%
Net present value ($1998)	$409,002,097

ES.1 ROLE OF NIST SRMS

Technical issues elevate the importance of accuracy and precision in the measurement of sulfur content. The primary environmental concern is sulfur dioxide (SO_2), which is produced from the combustion of fuels that contain sulfur as an impurity. SO_2 is directly harmful to health when inhaled and indirectly harmful because it generates acid rain. In addition to its detrimental impact on the environment, sulfur content also affects the quality of products and processes that use fossil fuels. For example, catalysts for low-emissions vehicles are sensitive to the sulfur content of gasoline and diesel fuel. Similarly, the catalysts used in petroleum processing can be "poisoned" by sulfur; sulfur affects the technical quality of other petroleum products as well. Fuel oils used in heat-treating metals or in firing glass-melting furnaces must be low in sulfur to avoid damaging the product. The sulfur content of coke has an impact on the quality of the steel it is used to produce.

Without NIST, the level of uncertainty associated with measuring sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the early 1980s.

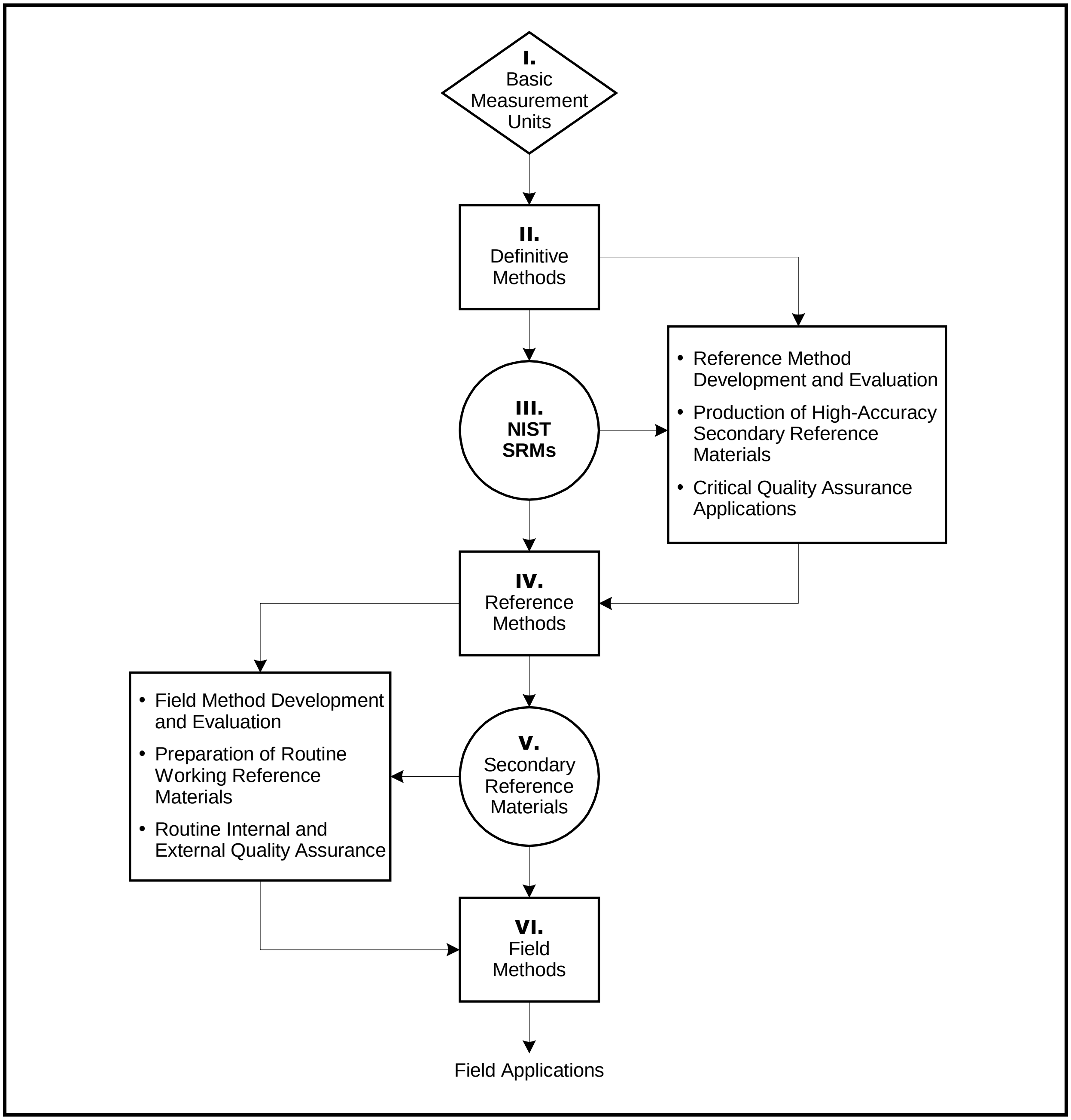
NIST's SRM program for sulfur in fossil fuels uses a definitive method, developed at NIST, that virtually eliminates bias and significantly reduces the uncertainty of the SRMs. Without the development of the isotope dilution thermal ionization mass spectrometry (IDMS) method, sulfur measurement in industry would be subject to greater bias and uncertainty. Because of the IDMS's complexity and the skill and equipment required, it is unlikely that any other laboratories developing certified reference materials (CRMs) would have pursued such a sophisticated method in the absence of NIST. Therefore, without NIST, the level of uncertainty associated with measuring sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the early 1980s.

Figure ES-1 illustrates the role that NIST SRMs play in the integrity of the measurement system. SRMs, which are tied to the basic measurement units maintained at NIST, are developed using IDMS. Many organizations use SRMs to develop and evaluate reference methods, to ensure the accuracy of secondary reference materials, and to ensure accuracy in critical quality assurance applications. Secondary reference materials and reference methods are then used to develop and evaluate field methods to prepare working reference materials, such as calibrants, and to perform routine quality assurance activities. The integrity of this system is based on the quality of NIST SRMs and their traceability to the basic measurement units.

Many companies and individuals benefit from the measurement improvements provided by NIST's sulfur in fossil fuels SRMs. We focused on those industries that make most extensive use of these SRMs and benefit most directly from their use. These companies use NIST SRMs in a variety of production stages, including

Figure ES-1. SRMs' Role in Measurement Accuracy

NIST SRMs play an integral role in users' quality control programs. They are used to develop and evaluate analytical methods, to produce secondary standards, and in quality assurance applications.



Source: Taylor, John K. February 1993. *Standard Reference Materials: Handbook for SRM Users.* NIST Special Publication 260-100. Washington, DC: U.S Government Printing Office.

marketing, applications development, production, and quality control. Industries include

- the sulfur measurement industry, including manufacturers of sulfur measurement instruments, CRMs, and independent laboratories that conduct sulfur analysis;
- the fossil fuels extraction and processing industry, including coal processing, petroleum refining, and coke production;[1] and
- primary users of fossil fuels, including the electric utility industry and the steel industry (see Figure ES-2).

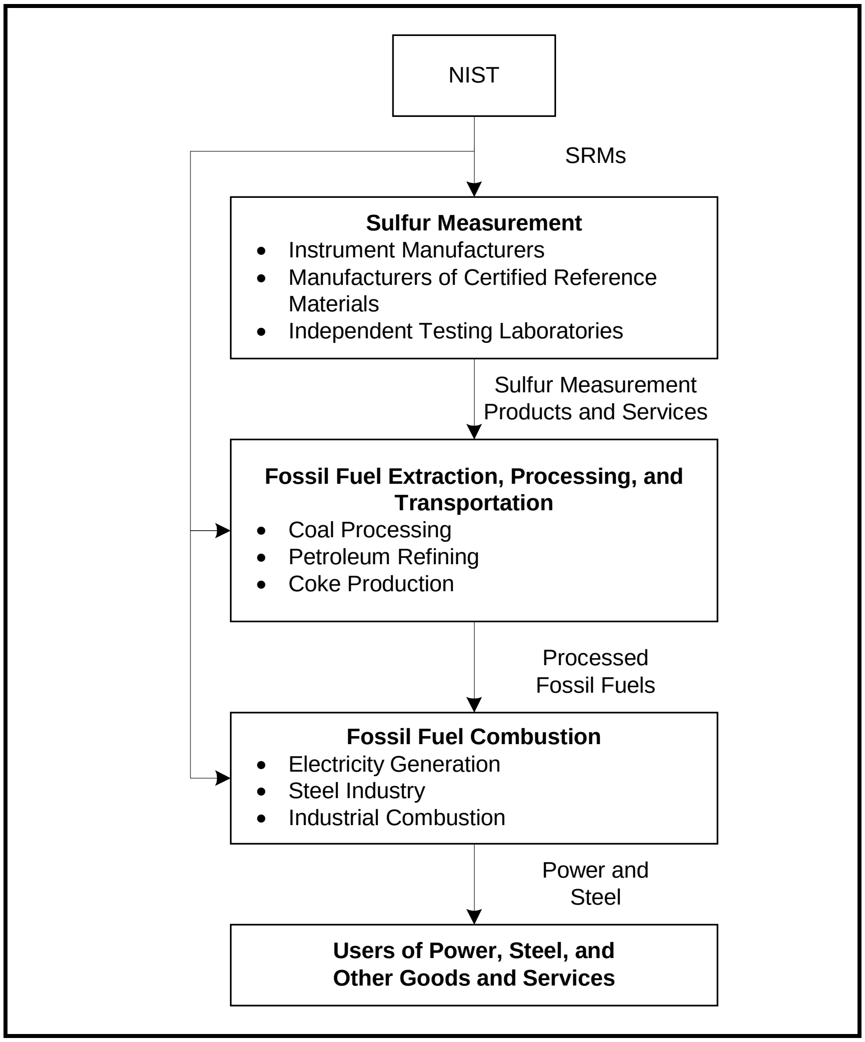


Figure ES-2. Industries Affected by Measurement of Sulfur in Fossil Fuels
Sulfur measurement is supported by each element of the measurement industry and is used by each member of the fossil fuel supply chain.

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[1] Although natural gas would normally be included in this characterization, we did not analyze the natural gas industry because NIST does not provide an SRM for sulfur in natural gas. As described in Appendix C, this is because very little sulfur is found in natural gas, and its measurement is not an important industry issue.

The potential impacts of these uses for sulfur information fall within the three categories of infratechnology impact discussed by Tassey (1997):

- **Infratechnologies improve the efficiency of R&D.** Sulfur SRMs reduce the cost of developing new products and processes in the sulfur measurement industry and in the fossil fuel industry.
- **Infratechnologies support the production process and enhance product characteristics.** Sulfur SRMs support quality control during the manufacturing and laboratory processes.
- **Infratechnologies reduce transactions costs.** SRMs allow these measurements to be made accurately and enable comparability among the results, thus promoting efficient and low-cost transactions.

Table E-2 summarizes our observations about how NIST SRMs may support production stages for each of the three industry sectors that we discuss. We used this general characterization of the role of infratechnologies in the economy and the potential role of NIST SRMs for sulfur in fossil fuels to develop hypotheses about how NIST SRMs affect each of the affected market segments.

Table ES-2. Potential Impact of SRMs on Stages of Production in the Sulfur Measurement Supply Chain

NIST SRMS may affect several stages of production for each industry segment.

	Stage of Production		
Industry Sector	**R&D**	**Production**	**Market Transactions**
Sulfur Measurement Industry	✓	✓	
Fossil Fuel Processing	✓	✓	✓
Fossil Fuel Combustion		✓	✓

ES.2 ANALYSIS RESULTS AND IMPACT CATEGORIES

The first step in quantifying the benefits from NIST sulfur SRMs is to develop a counterfactual scenario from which the benefits and costs can be measured. Our counterfactual scenario is that, in the absence of NIST, the level of uncertainty associated with measuring sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the early 1980s. Based on this counterfactual assumption, we are able to express the impact of NIST SRMs in terms of a change in the standard error (SE) of American Society for Testing and Materials (ASTM) sulfur measurement tests. Using the ratio of the old standard error to the new standard error and taking into account the percentage of measurement error associated with sampling, we estimate that NIST SRMs improve measurement accuracy by a factor of about 1.75 for petroleum and 1.25 for coal. These estimates allowed us to estimate possible economic impacts of sulfur SRMs.

We interviewed several members of each of the affected industries. Thirty-eight interviews were conducted with technical experts at 24 companies. The interviews were conducted in two stages: scoping interviews and technical interviews. During the scoping interviews, we learned about sulfur-content testing, methods and practices, and the importance of accurate sulfur-content information. We then used this information to develop and refine the questionnaire for the technical interviews. During the technical interviews, respondents were asked about sulfur testing and SRMs, their impressions of the impact of SRMs, and their use of the sulfur-content information.

We developed six hypotheses about the impact of NIST SRMs on industry, regulatory agencies, and the environment, and we evaluated them using data collected from primary and secondary sources. Table ES-3 summarizes the NPV of the benefits associated with the six hypotheses identified in this study. Of the six hypotheses, we were able to partially quantify the benefits for four hypotheses. Although we found anecdotal information to support the remaining hypotheses, little concrete evidence was available. Therefore, the potential benefits associated with these remaining hypotheses are discussed qualitatively, but they are not included in the estimates of economic return. In addition, industries' avoided expenditures on CRMs are included in the total benefit estimates.

Table ES-3. Net Present Value of Benefits and Costs
NIST expenditures of approximately $3.7 million lead to benefits of approximately $409 million.

	Benefits[a]	NIST Expenditures[a]
H1: Improved Product Quality	$2,665,422	
H2: Change in R&D Costs	–	
H3: Change in Transaction Costs	$7,542,201	
H4: Improved Production Efficiency	$401,408,574	
H5: Change in Regulatory Penalties	–	
H6: Benefits to Environment	$78,449,207[b]	
Avoided CRM Expenditures	$1,043,734	
NIST Investment Expenditures		$3,657,834
Total NPV ($1998)	$409,002,097	$3,657,834

[a] All benefits and costs are expressed as NPV ($1998).

[b] Not included in total NPV benefits summation.

The first hypothesis about the impact of SRMs on industry was that SRMs improve the quality of the products and services of the sulfur measurement industry, namely sulfur analysis equipment, CRMs, and sulfur analysis services. We were only able to quantify the impact on sulfur analysis services. Although CRM and instrument manufacturers said NIST SRMs affected their operations, interviewees were unable to quantify those impacts; thus, these areas are not included in the impact estimates in Table ES-3.

Our second hypothesis was that SRMs would reduce the cost of R&D to the sulfur measurement industry and the fuel industry by supporting accurate, reliable sulfur measurement. Although some of our interviewees indicated that NIST SRMs were part of their R&D laboratories' quality control program, they were not able to quantify any benefits to their R&D program from NIST SRMs.

Third, we hypothesized that NIST SRMs would reduce the cost of fossil fuel transactions because measurements are accepted as reliable; consequently, fewer transactions are disputed because of measurement error. Although most of our contacts indicated that, theoretically, better measurements would reduce the number of disputes, in actuality disputes seldom occur and only a small proportion of them are related to sulfur measurement problems.

We used information provided by industry to estimate the total cost of measurement disputes and assumed that 5 percent of that figure is the cost associated with measurement error.

Our fourth hypothesis was that NIST SRMs increase the efficiency of fuel blending, desulfurization, and equipment operations because the reliability of the measurement allows users to reduce the buffer they employ to ensure compliance with technical specifications. Petroleum refineries and coal companies are the primary beneficiaries of this impact because better sulfur measurement allows them to reduce the amount of desulfurization they conduct on fuels, which provides cost savings. Avoided desulfurization accounted for approximately 97 percent of the total benefits used to calculate measures of economic return.

Our fifth hypothesis was that improvements in the measurement of sulfur may reduce the incidence and quantity of penalties imposed by regulatory agencies. Thus, improved information on the sulfur content of products may lower the cost of production by lowering the cost of fines. Although industry experts agreed with this hypothesis, it was determined that fines paid by industry were in fact transfer payments and did not represent in themselves changes in social welfare. Thus, changes in regulatory penalties were not included in the benefit analysis.

The final hypothesis was that SRMs reduce the total amount of sulfur entering the environment by providing industry greater control over the sulfur content of its fuels and by allowing compliance officials greater authority in enforcing the regulatory limits. These benefits are not included in the total benefits presented in Table ES-3 or in the measures of economic return presented in Table ES-1 because they do not directly accrue to the sulfur measurement supply chain. As with the production efficiency hypothesis, the benefits to the environment associated with NIST SRMs are limited to petroleum products. With NIST SRMs, the reproducibility interval around the target sulfur content value is smaller, which means that batches of diesel fuel and gasoline are released with less sulfur. Lower sulfur fuels reduce the amount of SO_2 emitted to the environment. To estimate the economic impact, we valued the additional amount of SO_2 that would have been emitted to the environment in the absence of NIST SRMs.

In the absence of NIST SRMs, industry would likely purchase CRMs. Thus, avoided expenditures on CRMs are included as a benefit, offsetting NIST program expenditures.

The NPV of NIST's expenditures—including development, production, operation, overhead, and administrative costs—is $3,657,834. Based on the benefits we were able to quantify and NIST expenditures, the benefit-to-cost ratio associated with NIST/Technical Laboratories sulfur SRMs since 1984 is 113.

1

Introduction

The combustion of fossil fuels provides the majority of energy consumed in the U.S. This inexpensive and abundant source of energy is an integral part of the U.S. economy. Energy from fossil fuels has been and continues to be a key contributor to U.S. economic growth and productivity.

While the combustion of fossil fuels allows us to heat our homes, fuel our industries, and transport people and goods, it also has a negative effect on the quality of our environment. Sulfur dioxide (SO_2) gas and other sulfur compounds are emitted during combustion of fossil fuels that contain sulfur. These sulfur compounds have a detrimental effect on human health, wildlife, agricultural productivity, and quality of life and are a major contributor to acid rain. Sulfur compounds also reduce catalyst efficiency, increasing nitrogen oxide (NO_x) and hydrocarbon emissions from automobile engines. These negative environmental impacts have prompted the development of regulations that limit sulfur compound emissions from some sources and the sulfur content of some fuels. These regulations have evolved over time and have become more strict with respect to both sulfur content and sulfur compound emissions.

Sulfur in fossil fuels also affects the quality of a number of products. For example, catalysts for low-emissions vehicles are sensitive to the sulfur content of gasoline and diesel fuel. Similarly, the catalysts used in petroleum processing can be "poisoned" by sulfur; sulfur affects the technical quality of other petroleum products as well. Fuel oils used in heat-treating metals or in firing glass-melting furnaces must be low in sulfur to avoid damaging the product. The sulfur content of coke has an impact on the quality of the steel it is used to produce.

Because sulfur has a negative effect on both the environment and on the quality of products, low-sulfur fuels are more desirable than high-sulfur fuels. However, because low-sulfur fuels are scarce and removing sulfur from fossil fuels is expensive, low-sulfur fuels are more valuable than high-sulfur fuels. The sulfur content of fossil fuels has become increasingly important to the value of these fuels as environmental regulations gradually lower the sulfur content limits for fossil fuels and restrict the emission of sulfur from fossil fuel combustion. These regulations have encouraged the development of technologies that remove sulfur from fossil fuels and the design of transportation and power generation equipment that operate on low-sulfur fuel.

Because sulfur is a key characteristic of fossil fuels and an important factor in determining their value, information about the sulfur content of fossil fuels is important to industry This information is used by industry in three ways:

- Sulfur content information is used to write and execute fossil fuel purchase contracts. It supports the millions of fuel transactions that occur in the U.S. every year.
- Sulfur content information is used during fuel extraction, blending, and processing operations to improve their efficiency. An accurate measure of the sulfur content allows companies to meet strict product specifications.
- Sulfur content information is used by industry and by the regulatory community to ensure that fuels meet sulfur content regulations and that their combustion will not violate an emissions permit.

The National Institute of Standards and Technology (NIST) promotes U.S. economic growth by working with industry to develop and apply technology, measurements, and standards. NIST, through its Office of Standard Reference Materials, is authorized to certify and sell standard reference materials (SRMs). SRMs are materials certified for their chemical composition or physical properties; they are developed by various laboratories at NIST. SRMs help users verify the accuracy of measurement methods or calibrate measurement systems by linking their measurements to NIST. The development of SRMs employs NIST's unique experience in measurement. A NIST-certified SRM carries with it the full weight and authority of NIST and the U.S. Department of Commerce.

Among the approximately 1,300 SRMs available from NIST, 27 are SRMs for measuring sulfur in fossil fuels. These SRMs and the methods used to certify them are developed by NIST's Technical Laboratories. As emerging regulations increase the importance of the sulfur content of fossil fuels, NIST is expanding its suite of fossil fuel SRMs to include SRMs for measuring sulfur in the low-sulfur fuels that are required to meet these regulations.

To provide input to NIST's program planning and evaluation process, Research Triangle Institute (RTI) conducted a study to identify, characterize, and quantitatively estimate the economic impact of NIST's SRMs for sulfur in fossil fuels. This report describes the study and discusses our conclusions.

1.1 NIST'S SRM PROGRAM FOR SULFUR IN FOSSIL FUELS

All measurements depend on standards. Chemical measurements, such as the measurement of sulfur in fossil fuels, depend on both physical standards and chemical standards. Although early chemical analytical measurements depended almost entirely on physical standards, modern techniques rely more heavily on chemical standards. This is because most modern chemical measurements rely on comparative techniques by which an instrument is used to compare an unknown sample with one of known composition (Taylor, 1993).

SRMs play a key role in the National Measurement System for Analytical Chemistry. They serve as national primary chemical standards and are used as calibrants and as quality assurance materials to evaluate measurement accuracy, to intercalibrate laboratories in a measurement program, and to provide compatibility of measurement data (Taylor, 1993). If SRMs as primary chemical standards did not exist, the entire national measurement infrastructure would be weakened.

NIST's SRM program for sulfur in fossil fuels began in 1968 with the certification of two residual fuel oil standards, SRMs 1621 and 1622, which contain 1 and 2 percent sulfur, respectively. The sulfur content for both of these SRMs was certified using a gravimetric method similar to American Society for Testing and Materials (ASTM) D-129 (General Bomb Method). In the early 1980s, scientists at NIST (in particular, Paulsen and Kelly [1984]) began developing an application of isotope dilution mass spectrometry (IDMS) to the certification of sulfur in fossil fuels. IDMS is now considered a definitive method that virtually eliminates bias in the certified value. It has significantly reduced the uncertainty associated with the certified values, providing a more reliable standard for all laboratories testing the sulfur content of fossil fuels.

Today, the importance of sulfur content measurement for fossil fuels is growing as the U.S. Environmental Protection Agency (EPA) continues to reduce the allowable sulfur in fuels and the auto industry moves toward lower emissions vehicles that use catalysts that are even more sensitive to sulfur in fuels. NIST SRMs will continue to play an important role in the measurement system for sulfur in fossil fuels. For example, NIST recently developed SRMs for sulfur in reformulated gasoline (RFG). RFG is required in nine metropolitan areas of the U.S. as part of the 1990 Clean Air Act. Two of these SRMs are certified at very low sulfur levels, consistent with the low sulfur content currently required in California and on the horizon nationally. NIST will continue to issue SRMs as industry expresses the need for standards that support the analysis of sulfur content in ultra-low sulfur fuels.

1.2 PROJECT OBJECTIVES AND SCOPE

The objective of this project is to identify, characterize, and quantitatively estimate the economic impact of NIST's SRMs for sulfur in fossil fuels on the relevant industries. We need to understand how the sulfur content of fossil fuels affects the economy and how information about sulfur content affects the economic decisions of agents in the economy. By modeling those decisions, we can quantify how the world would be different in the absence of the NIST SRMs that improve the accuracy and precision of these measurements.

NIST's SRM program includes over 1,300 SRMs. For this project, we examined only the 29 SRMs shown in Table 1-1. Each of these SRMs supports measurement methods used to determine the sulfur content of fossil fuels.

Table 1-1. NIST SRMs Covered by this Study

This study examines the impact of 27 existing SRMs and two SRMs that were still under development in early 1999.

SRM Number	Description	First Certificate Date[a]	Years of Reissue
1616	Sulfur in Kerosene	2/19/88	1995
1617	Sulfur in Kerosene	2/19/88	1995
1619	Sulfur in Residual Fuel Oil, 0.7%	12/22/81	1991, 1998
1620	Sulfur in Residual Fuel Oil, 4%	12/1/79	1981, 1990
1621	Sulfur in Residual Fuel Oil, 1%	12/11/67	1980, 1981, 1986, 1991, 1996
1622	Sulfur in Residual Fuel Oil, 2%	12/11/67	1979, 1981, 1986, 1991, 1997
1623	Sulfur in Residual Fuel Oil, 0.3%	4/7/71	1981, 1990, 1996
1624	Sulfur in Distillate Fuel Oil, 0.4%	4/7/71	1981, 1990, 1997
1819	Sulfur in Lubricating Base Oil	7/17/85	1994
2294	Reformulated Fuels (nom. 11% MTBE, 35 mg/kg sulfur)	3/10/98	
2295	Reformulated Fuels (nom. 15% MTBE, 300 mg/kg sulfur)	3/10/98	
2296	Reformulated Fuels (nom. 13% ETBE, 35 mg/kg sulfur)	3/10/98	
2297	Reformulated Fuels (nom. 10% Ethanol, 300 mg/kg sulfur)	3/10/98	
2717	Sulfur in Residual Fuel Oil	10/25/90	
2718	Green Petroleum Coke	7/15/99	
2719	Calcined Petroleum Coke	7/15/99	
2724	Sulfur in Distillate Fuel Oil, 0.04%	8/17/92	1995
1632	Trace Elements in Coal (Bituminous)	3/7/75	1978, 1998
1633	Trace Elements in Coal Fly Ash	3/7/75	1979, 1993
1635	Trace Elements in Coal (Subbituminous)	10/24/95	
2682	Sulfur in Coal, 0.5%	12/14/82	1998
2683	Sulfur in Coal, 2%	12/14/82	1992, 1997
2684	Sulfur in Coal, 3%	12/14/82	1992
2685	Sulfur in Coal, 5%	12/14/82	1994
2690	Trace Elements in Coal Fly Ash	12/20/93	
2691	Trace Elements in Coal Fly Ash	12/20/93	
2692	Sulfur in Coal, 1%	11/15/88	1994
2775	Foundry Coke	5/12/99	
2776	Furnace Coke	3/19/98	

[a] The first certificate date indicates the date that the certificate was issued for the first batch of this SRM. As new batches are developed, new certificates are issued and the SRM is redesignated with an appropriate letter after the number signifying which batch it is from. For example, SRM 1632a was the second batch of 1632; SRM 1632b was the third batch of 1632.

Many companies and individuals benefit from the availability of SRMs that improve the measurement of the sulfur content of fossil fuels. We focused on those industries that make the most extensive use of these SRMs and benefit most directly from their use. These industries include

- the sulfur measurement industry, including manufacturers of sulfur measurement instruments, certified reference materials (CRM), and independent laboratories that conduct sulfur analysis;
- the fossil fuels extraction, processing, and transportation industry, including coal processing, petroleum refining, and coke production;[1] and
- primary users of fossil fuels, including the electric utility industry and the steel industry. Industrial combustion also accounts for a large percentage of the fossil fuels consumed in the U.S. However, because of the difficulty of characterizing the diverse set of industries that engage in industrial combustion, we did not address industrial combustion in this study.[2]

1.3 SUMMARY OF ANALYTICAL APPROACH AND REPORT ORGANIZATION

NIST SRMs support the measurement of sulfur in fossil fuels. These measurements are provided by a sulfur measurement industry and support economic activity in the entire fossil fuel supply chain. To estimate the economic impact of SRMs for sulfur in fossil fuels on these industries, we employed a methodology that allowed us to value the economic outcomes resulting from decisions that use the improved information provided by NIST SRMs. Figure 1-1 provides an overview of this method. First, we examined how NIST SRMs affect the measurement of sulfur in fossil fuels, including the accuracy of these estimates and the cost of conducting these tests. Second, we evaluated how improvements in measurement quality provided by NIST SRMs affect the behavior of people and

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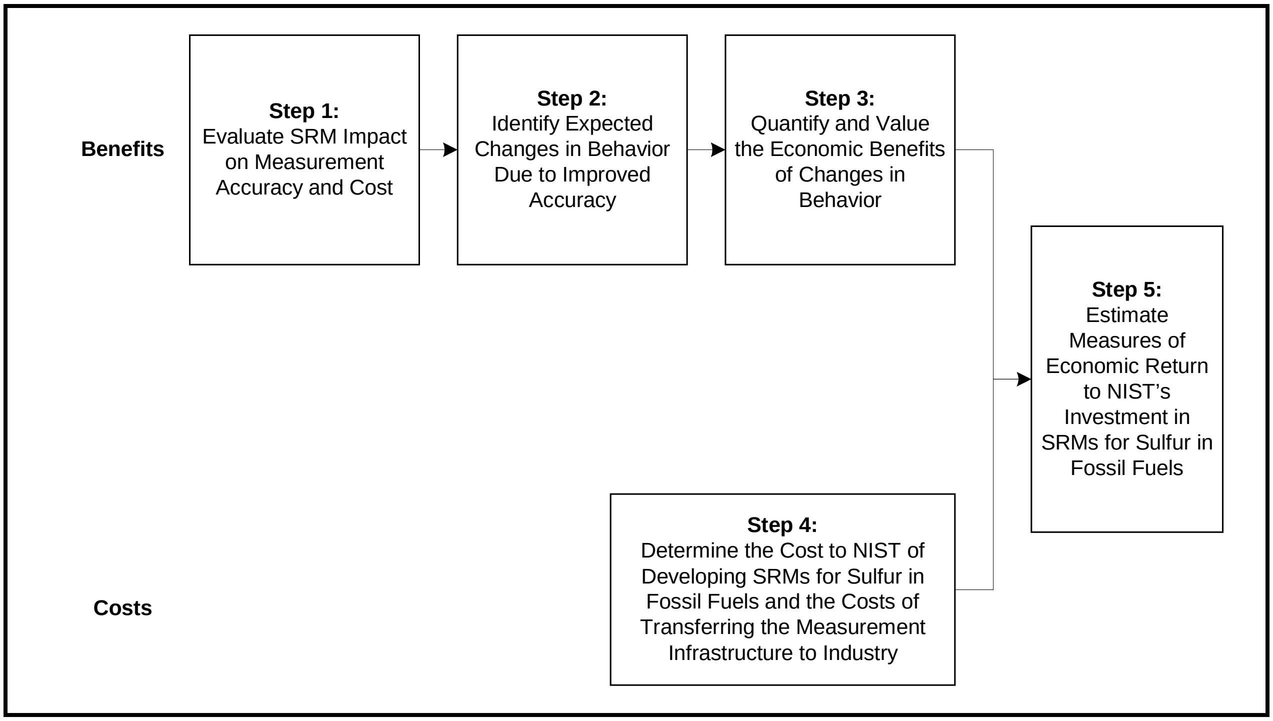
[1] Although natural gas would normally be included in this characterization, we did not analyze the natural gas industry because NIST does not provide an SRM for sulfur in natural gas. As described in Section 2, this is because very little sulfur is found in natural gas, and its measurement is not an important industry issue.

[2] Industrial combustion refers to the use of industrial, commercial, and institutional (ICI) boilers whose primary use is for process heating, electrical or mechanical power generation, and/or space heating.

Figure 1-1. Analytical Approach to Assessing the Impact of NIST's Technical Laboratories Sulfur in Fossil Fuel SRMs

This five-step analytical approach captures the benefits and costs of NIST's SRMs for sulfur in fossil fuels.



companies that use sulfur content measurements. Third, we quantified and valued the economic benefits of these changes in behavior to provide a numerical estimate of the benefits of the NIST SRMs. We then compared those benefits with the costs of the SRM program and estimated measures of economic return to society's investment.

This report is organized into seven sections. Section 2 provides background on the industries affected by the measurement of sulfur in fossil fuels and contains some of the basic economic information needed to conduct our analysis. Section 3 describes how sulfur in fossil fuels is measured, why these measurements are subject to error, and how NIST's SRM program has improved the measurement of sulfur in fossil fuels over time. Section 4 describes our approach to valuing improvements in the accuracy of the measurement of sulfur in fossil fuels. It explains how sulfur information affects industry, lists our hypotheses for the study, and describes impact measures for quantifying technical and economic impacts. It also describes the data we used to conduct the analysis and the data collection process. Section 5 describes the results of the study, carefully reviewing the evidence to support or refute each of the hypotheses developed in Section 4. Section 6 explains why NIST has played, and will continue to play, such an important role in the development of these SRMs. Section 7 offers conclusions based on our analysis and observations about the role of NIST SRMs in industry.

2

Overview of Affected Industries

The combustion of fossil fuels provides 85 percent of the energy consumed in the U.S. Each year U.S. households and industry consume 1 billion tons of coal, 7 billion barrels of oil, and 20,000 cubic feet of natural gas (U.S. DOE, 1998a). Fossil fuels affect virtually every sector of the U.S. economy because they provide the power required to manufacture goods; heat and cool homes, offices, and factories; provide services; and transport people and goods.

Sulfur is an important factor in determining the value of fossil fuels. Increasingly strict environmental regulations limit the sulfur content of some fuels and also limit sulfur compound emissions that result from its combustion. Sulfur also has a negative impact on the quality of some products and processes. Removing sulfur from fossil fuels is expensive, and the natural sulfur content of these fuels is increasing.

Because sulfur is an important determinant of the value of fossil fuels, an accurate measurement of the sulfur content of fossil fuels and of downstream products is essential to support commerce. These measurements also help industry demonstrate regulatory compliance and control the quality of their products.

NIST SRMs facilitate measurements and standards throughout the fossil fuel supply chain. The measurement industry uses NIST SRMs to verify the quality of their instruments' calibration, reference materials, and measurement procedures. The fossil fuel extraction companies and their customers use NIST SRMs similarly to verify the quality and reliability of the measurements they make for transactions, process control, and environmental compliance. The regulatory community uses SRMs to ensure environmental compliance by the regulated industries.

Figure 2-1 illustrates the relationships among the industries in the supply chain. Appendix C contains profiles of the industries that use SRMs to measure sulfur content. It describes the importance of sulfur as a characteristic of fossil fuels; includes a profile of the affected industries; and describes how NIST SRMs support these industries.

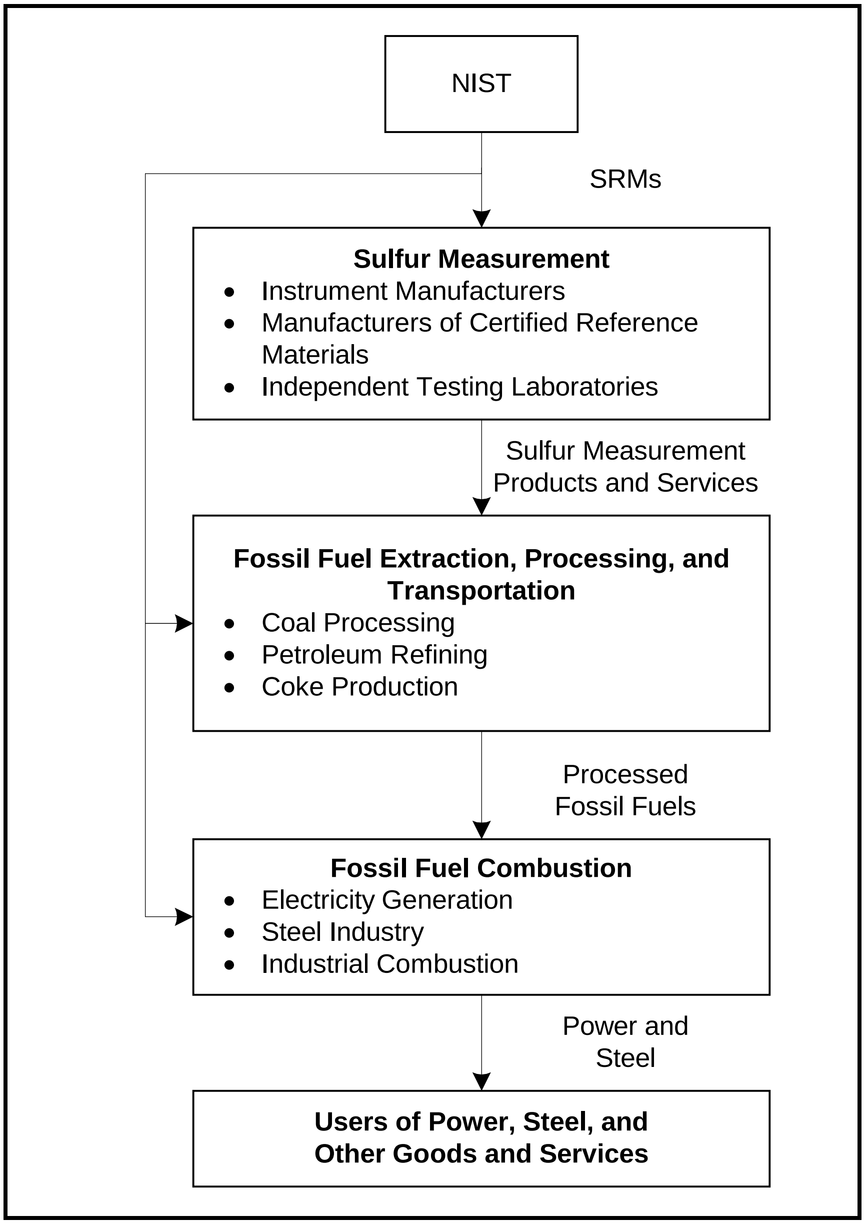


Figure 2-1. Industries Affected by Measurement of Sulfur in Fossil Fuels
Sulfur measurement is supported by each element of the measurement industry and is used by each member of the fossil fuel supply chain.

This section provides an overview of the key industries discussed in Appendix C. Although many industries engage in the measurement of sulfur content, we concentrated on three sectors—sulfur measurement industry, coal processing, and petroleum refining—because they are primary users of SRMs for their in-house sulfur measurement activities.[1]

2.1 SULFUR MEASUREMENT INDUSTRY

The industry that supports the measurement of sulfur in fossil fuels includes the manufacturers of instruments, suppliers of CRMs, and independent laboratories that conduct sulfur analysis.

2.1.1 Instrument Manufacturers

Determinators, spectrometers, elemental analyzers, and chromatographers are measurement equipment used to determine the elemental composition of organic and inorganic samples. Manufacturers and consumers of these measurement instruments use NIST's sulfur SRMs to test and calibrate their equipment. These instruments must be properly calibrated to provide quality laboratory results. Sulfur SRMs allow technicians to test an instrument's accuracy and inform them of any need for adjustments. Equipment technicians may use NIST's sulfur SRMs directly, or they may use NIST-traceable CRMs from a secondary manufacturer to calibrate laboratory equipment.

2.1.2 Manufacturers of Certified Reference Materials

A certified reference material (CRM) is defined by the International Standards Organization (ISO) as "a reference material one or more of whose property values are certified by a technically valid procedure, accompanied by or traceable to a certificate or other documentation which is issued by a certifying body" (American National Standards Institute [ANSI], 1981). CRMs are used in the same way as NIST SRMs—for equipment calibration, development of other standards, and quality control for analyzing sulfur in fossil fuels. CRMs are often used in conjunction with NIST SRMs. In many laboratories, CRMs are used on a daily basis while NIST SRMs are used only occasionally.

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[1] Appendix C also contains an overview of the coke, electricity, and steel industries and discusses sulfur measurement issues related to these industries.

CRMs are generally prepared using NIST SRM products (when available) and ASTM procedures. However, none of the CRM producers duplicate the procedures followed by NIST. NIST SRMs for sulfur in fossil fuels are certified using a technique known as IDMS. As explained in Section 3, IDMS is a definitive method that virtually eliminates bias and significantly reduces the relative uncertainty associated with reference materials. No commercial CRM manufacturers use IDMS; instead, they employ ASTM methods and/or interlaboratory testing for certification. The less rigorous process used by the CRM manufacturers can sometimes lead to significant differences between the accuracy and precision of the certified values provided by NIST and those provided by a CRM manufacturer.

Traceability ensures that secondary standards, such as CRMs, can be linked to national standards. However, the length of the pathway from the user of a measurement back through intermediate calibration to national standards or fundamental constants has an important effect on the level of uncertainty of the measurement. With each transfer point along the traceability pathway, the accuracy of the measurement degrades because each laboratory introduces its own measurement error to the process. Furthermore, it is not always a simple matter to interpret the uncertainty measurements provided by intermediate laboratories. For this reason, it is generally presumed that a shorter traceability pathway is preferred when uncertainty must be minimized or when knowledge of uncertainty is important (Garner and Rasberry, 1993).

2.1.3 Independent Sulfur Testing Laboratories

Independent sulfur testing laboratories fall within SIC 8734, Testing Laboratories. In 1992, the U.S. had over 4,500 commercial testing laboratories generating almost $5 billion in revenue and $2 billion in payroll each year (U.S. DOC, 1994).[2] A small subset of these laboratories conducts sulfur analysis of fossil fuels. These laboratories provide inspection, sampling, and analytical services for fossil fuel producers and consumers.

Independent laboratories are an important link in the supply chain affected by SRMs. Although many mines, coking plants, coal preparation plants, utilities, and refineries have their own laboratories for these analyses, independent laboratories are becoming more important, particularly for contractual matters. Third-party independent laboratory results are routinely used to satisfy contractual requirements for buyers and sellers in the coal industry, and this arrangement is increasing in the petroleum industry as well. To cut costs, some firms also hire independent laboratories rather than operate their own.

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[2] These figures include taxable firms only. Noncommercial research organizations are not included.

2.2 COAL INDUSTRY

The U.S. coal industry produces and distributes 1.1. billion short tons of coal per year. The industry consists of a few very large companies that produce more than 50 percent of total coal production and many mid-size and small companies. Information about the sulfur content of coal is very important to this industry because the price of coal is a function of its sulfur content among other attributes. Removing sulfur from coal is expensive, and the sulfur content of coal determines whether an electric utility plant that burns it can meet its regulatory emissions requirements for SO_2.

Coal is generally classified into four sulfur categories: compliance, low sulfur, medium sulfur, and high sulfur. Compliance coal has the lowest sulfur content—0.6 pounds per million Btus or less. It naturally falls within federal emissions regulations and therefore requires less cleaning before combustion. Low-sulfur coal has between 0.61 and 1.25 pounds of sulfur per million Btus, medium sulfur coal between 1.26 and 1.67 pounds per million Btus, and high-sulfur coal more than 1.67 pounds per million Btus.

Coal's sulfur content varies by the location from which it is mined. Generally, western coal (from Colorado, North Dakota, and Wyoming, for example) is lowest in sulfur; Appalachian coal (from Pennsylvania, West Virginia, and Kentucky, for example) is either low or medium sulfur; and interior coal (from Indiana, Illinois, Ohio, for example) is medium and high sulfur.

2.2.1 Coal Cleaning and Processing

Coal processing entails the mining, cleaning, and distribution of coal from underground and surface mines. Figure C-4 in Appendix C provides an overview of activities, inputs, and outputs of the coal processing industry.

Coal is extracted from two categories of mines: underground and surface mines. Underground coal mining entails cutting a slot, known as a kerf, at the bottom of a face; drilling holes in the face for explosives or compressed air; blasting the coal; and loading and hauling it out of the working area to a conveyor belt or mine cars (Pennsylvania Department of Environmental Protection, 1999). Surface mining refers to the removal of dirt and rock on top of a coal seam so that it can be excavated, placed on conveyors, and sent to preparation plants. Strip mining is the most popular surface mining method in the U.S.

On-site coal preparation plants make coal more valuable through size reduction, desulfurization, and removal of moisture and inorganic impurities. Nearly 50 percent of the coal mined in the U.S. passes through coal preparation plants; east of the Mississippi River this number increases to 80 percent (Fonseca, 1995). Coal preparations, which "clean" coal by removing impurities, may account for 5 to 15 percent of the cost of coal production (Horton and Bloom, 1993).

Coal preparation plants remove coal mechanically by taking advantage of differences between the impurities and the coal's density. Water is used to fluidize a bed of crushed coal and its contaminants. As the lighter coal particles float to the top, the impurities are separated. The coal is then skimmed off the top of the bed and dried using a combination of hot gases. Coal is also blended to meet customer specifications. For example, high- and low-sulfur coal can be mixed together as part of the preparation and cleaning process to ensure the sulfur content of the delivered coal meets sulfur levels specified in contracts.

2.3 PETROLEUM INDUSTRY

The U.S. petroleum industry supplies over 6 billion barrels of petroleum products per year. The industry is dominated by a small number of large, vertically integrated companies. This structure is driven by the large capital costs associated with the petroleum refining technology.

The main determinants of crude oil prices are sulfur content (sweet versus sour) and API gravity (light versus heavy). High API gravity, or light crude, is more valuable because it is used in more high-end products when distilled and has fewer impurities. Sulfur information allows refineries to control the sulfur content of output streams and emissions. Both are required for regulatory compliance

The composition of crude oil varies greatly from field to field throughout the world. For example, Alaskan crude typically has a low sulfur content (sweet), and South American crude typically has a high sulfur content (sour). Crude oil with a high sulfur content is more expensive to refine because it is difficult to separate sulfur compounds from pure hydrogen/carbon compounds (Leffler, 1985).

2.3.1 Petroleum Processing and Desulfurization

Petroleum refining is the physical, thermal, and chemical separation of crude oil into its major distillation fractions, which are then further processed through a series of separation and conversion steps into finished petroleum products and chemical industry feedstocks.

Sulfur is removed from petroleum products by reacting it with hydrogen gas in the presence of a catalyst at a moderately high temperature and pressure. This process is referred to as hydrodesulfurization or hydrofinishing. In addition to desulfurization of final products, sulfur recovery for sale of elemental sulfur is also conducted for refinery process off-gas streams as part of emissions reduction activities. The sulfur is converted to hydrogen sulfide, which is then absorbed through desulfurization of stack gases.

Desulfurization of petroleum output streams can be very expensive. As part of background research for the development of its new sulfur content in gasoline regulations, EPA developed estimates of the cost of removing sulfur from gasoline. As shown in Table C-16 in Appendix C, for example, reducing the sulfur content of gasoline from 330 ppm to 40 ppm costs about 1.6 cents per gallon.[3]

Maintaining specific sulfur levels in output streams and process off-gas streams is difficult because of the varying content of sulfur in crude oil. Accurate information about the sulfur content of the crude oil and the output streams is essential to maintaining product specifications and maximizing the efficiency of the processing equipment.

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[3] The American Petroleum Institute (API) believes that EPA underestimated the added cost of reducing the sulfur content of gasoline below current levels. The trade association funded a series of studies conducted by MathPro that estimated the cost to be 2.3 to 2.6 cents per gallon (*Octane Week*, 1999). Although API's estimates are provided in Table C-16, the economic estimates presented in this study are based on the more conservative EPA estimates of approximately 1 cent per gallon.

3 SRMs and Sulfur Measurement

To assess the economic impact of SRMs on the affected industries, we must first assess the impact of NIST SRMs on the accuracy of sulfur content measurement. In this section, we demonstrate that NIST SRMs are responsible for reducing the bias and improving the precision of sulfur content measurement in industry. We quantify the relationship between NIST SRMs and sulfur measurement accuracy and use this relationship in the next stage of the analysis.

We begin by describing the sources of variability in measurement and how this variability is quantified. Then we describe the ASTM methods used most frequently to measure the sulfur content of fossil fuels, including the role of reference materials in these methods. We explain how bias and uncertainty in a reference material introduce bias and uncertainty into the measurement process. In Section 3.3, we describe the process of SRM development and the history of the NIST SRM program for sulfur in fossil fuels. We demonstrate the relationship between NIST's methodology development and the reduction in uncertainty and bias associated with the certified values of NIST SRMs. Finally, we conclude that, in the absence of the NIST SRM program, the accuracy of measurements of sulfur in fossil fuels would today be similar to what it was prior to the introduction of new NIST methods in the early 1980s.

3.1 UNCERTAINTY IN THE MEASUREMENT OF SULFUR IN FOSSIL FUELS

All measurements, including measurements of the sulfur content of fossil fuels, are subject to some uncertainties. The measured value of a variable is a function of both its true value and the measurement system. The measurement system contains a number of elements that contribute to uncertainty in measurement (Taylor, 1997; Bentley, 1983). Uncertainties of analytical measurements must be quantified so that decision-makers can understand the degree of reliability of the result. NIST SRMs play a role in both reducing and quantifying the uncertainty of field laboratory measurements.

3.1.1 Sources of Variability in Measurement

A number of factors contribute to uncertainty in measurement. NIST defines accuracy as the closeness of a measured value to the true value. Accuracy is a "relative" measure and includes both the concepts of precision and bias. Precision refers to the variability of individual results of replicate measurements. Bias is the difference between the observed mean of those measurements and the true mean (Taylor, 1993).

The ASTM defines the sources of variability of a measurement method, each of which belongs to one of the following categories:[1]

- the operator
- the apparatus
- the environment
- the sample
- time

The operator must interpret the test method and execute it. The greater the clarity of the test method, the less it is open to incorrect interpretation. Different operators (and the same operator at different times) introduce variability into the process because of differences in dexterity, reaction time, color sensitivity, ability to interpolate scale readings, and so forth.

Apparatus typically allow variations in measurements due to specification tolerances. Because no apparatus can be built that has zero tolerance, these variations are one source of variability between test results from different test equipment. Apparatus calibration is also a potential source of error. An instrument that is not calibrated correctly or is calibrated to an incorrect standard

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[1] This section is taken from ASTM Method E 177.

may introduce bias into the measurement process. NIST SRMs for sulfur in fossil fuels directly impact this potential source of bias.

The environment also contributes to measurement uncertainty. Although test methods typically specify the standard environmental conditions for testing, these factors cannot be controlled perfectly. Thus, slight differences in environment yield differences in test results.

Another source of uncertainty is sampling. A batch or lot of material to be tested (such as a shipment of coal or tank of fuel) is rarely perfectly uniform. Sampling methods are typically employed to ensure that the sample is representative of the lot; however, sampling is often (especially in the case of coal, which is typically very heterogeneous) a large source of measurement uncertainty.

All of the above sources of uncertainty in measurement can change over time, and this contributes to variability in measurement. For example, the environment in a laboratory may change systematically over time. Thus, the longer the amount of time between different realizations of a test method, the greater the potential variability in the results.

These sources of uncertainty suggest strategies to reduce uncertainty in the measurement process. Variability due to the operator can be reduced by providing clear, complete instructions to operators regarding the proper methodology. Careful training and quality control in the execution of the method might also reduce the uncertainty associated with the test method.

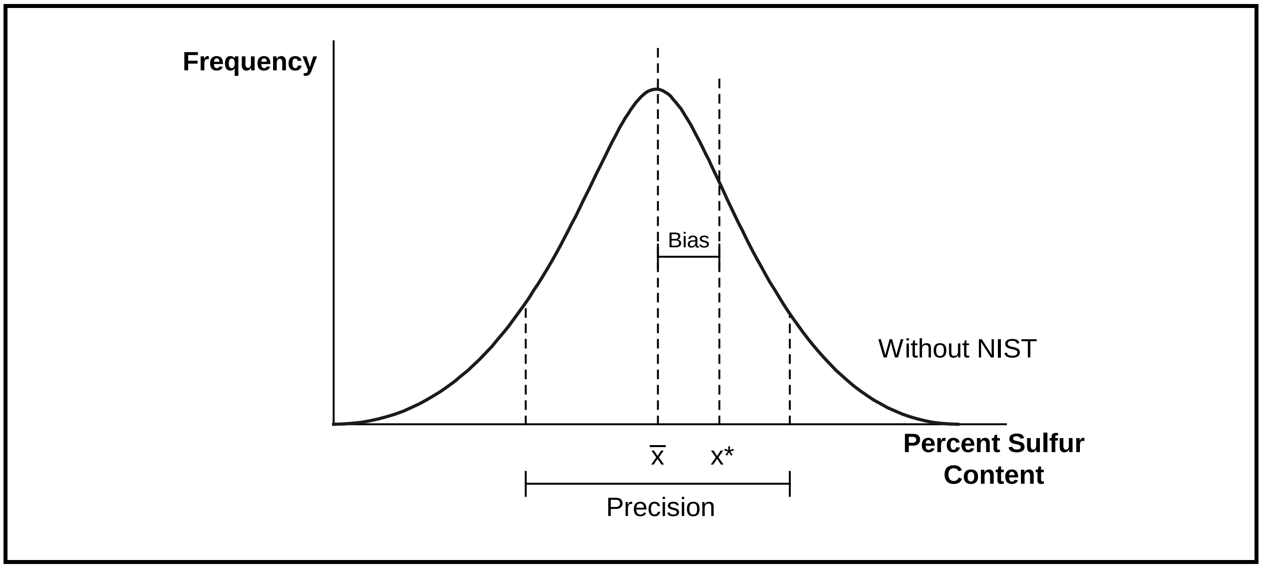
Uncertainty due to the apparatus can be reduced by improving the instrument's tolerances, by more careful (or more frequent) calibration and quality control of the instrument, or by calibration to a more reliable standard. Calibration to a more reliable standard and the ability to perform quality control against a known is perhaps the primary contribution of NIST SRMs to reducing uncertainty in measurement. They also allow the bias and precision of a measurement process to be quantified.

Variability due to the environment can be reduced by carefully controlling the conditions under which measurements are made. Uncertainty due to the sample can be reduced by taking more samples or by taking more composites of a sample.

3.1.2 Quantifying the Uncertainty of a Measurement Process

We can describe two aspects of uncertainty associated with a measurement: bias and precision. These concepts are illustrated in Figure 3-1 and discussed below.

Figure 3-1. Bias and Precision in Test Methods
Bias is the difference between the mean of a set of test results ($\bar{x}$) and the accepted value (x*); precision is a measure of the dispersion of the test results.



One important contribution of NIST SRMs is the establishment of a reference value so that the bias of a measurement method can be determined. An analyst can then compensate for the measurement method's bias.

The *bias* of a measurement process describes the relationship between the test results from the process and an accepted reference value. The bias of a measurement process is determined by taking the average of a large set of test results ($\bar{x}$) and comparing it against the accepted reference value. In Figure 3-1, if x* is the accepted reference value, then the bias of the measurement system is $|\bar{x} - x^*|$.

If an accepted reference value is not available, the bias cannot be established. The accepted reference value is a value that serves as an agreed-upon reference for comparison. It may be a theoretical or established value based on scientific principles (which is sometimes called the "true" value), or it may be an assigned or consensus value based on experimental work. The certified values of a NIST SRM are universally accepted reference values.

If the bias in a test method is known, an adjustment for the bias can be incorporated into the test method. Thus, one important benefit of having an accepted reference value is the ability to assess and adjust for the bias.

The *precision* of a test method refers to the closeness of agreement among multiple test results obtained under similar conditions. The greater the dispersion of the results, the poorer the precision. Two different types of precision are commonly determined for a test method. *Repeatability* (r) is determined by conducting the method repeated times under similar conditions within a single laboratory, by the same operator, with the same equipment, in the shortest practical period of time. *Reproducibility* (R) is determined from the results of tests obtained in different (independent) laboratories under similar conditions.

The standard deviation (denoted by s) of an ASTM method can be determined from the stated 2s interval by dividing the interval in half and then dividing it by 1.96. Similarly, s can be determined from the d2s interval by dividing the interval in half and then again by $1.96\sqrt{2}$.

Precision is often expressed as an index in the same units as the test result. These indexes are related to the estimate of the sample standard deviation, s, of a random set of test results. The two indexes of precision used most commonly by the ASTM for sulfur in fossil fuels are as follows:

- *Two Standard Deviation Limits (2s).* This measure of precision refers to an interval that expresses the dispersion of individual test results in relation to the average value. Ninety-five percent of individual test results from similar labs will differ from the average value in absolute value by less than 1.96 s. In Figure 3-1, if $\bar{x}$ is the average of results of an interlaboratory study, then 95 percent of individual test results from similar labs will fall within the interval $\bar{x} \pm 1.96$ s.
- *Difference "Two" Standard Deviation Limit (d2s).* This measure of precision refers to the dispersion of pairs of test results relative to each other. In Figure 3-2, suppose x_1 and x_2 are a pair of test results from laboratories similar to those in the study. In 95 percent of all pairs, x_1 and x_2 will differ in absolute value by less than $1.96\sqrt{2}$ s.[2]

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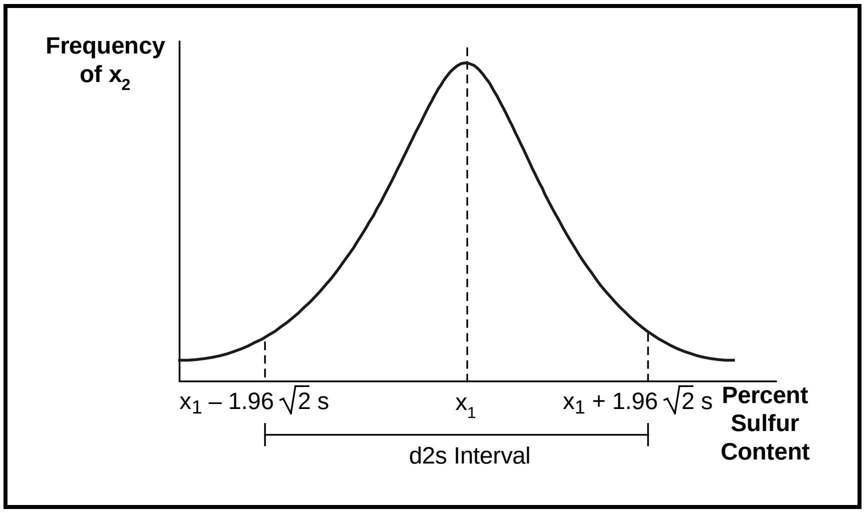
[2] If the variance of an observation x is equal to s^2, then the variance of a difference in such observations, if they are uncorrelated, will be $2s^2$; $\mathrm{Var}(x_1 - x_2) = \mathrm{Var}(x_1) + \mathrm{Var}(x_2) = 2s^2$. Hence, the standard deviation of the difference will be $\sqrt{2}s$, and the interval estimate to contain 95 percent of such differences will be $1.96\sqrt{2}s$.

Figure 3-2. Difference "Two" Standard Deviation Limit (d2s)
Any pair of test results, X_1 and X_2, will lie within the d2s interval 95 percent of the time.



3.2 METHODS FOR MEASURING SULFUR IN FOSSIL FUELS

Although a number of methods exist for measuring sulfur in fossil fuels, industry relies increasingly on instrumental methods that require the use of calibrants. The accuracy of these methods depends a great deal on proper calibration and quality control procedures. NIST SRMs provide a reference material that can be used as a calibrant, a check on the true value of a calibrant, and a quality control material for ensuring that the method is providing accurate results.

This section provides a brief description of these methods and describes the importance of NIST SRMs in ensuring their accuracy. The first section reviews the most common methods for measuring sulfur in coal. The second section reviews the most common methods for measuring sulfur in petroleum products. The last section describes the statistical relationship between the accuracy of the certified value of a reference material and the accuracy of the sulfur content measurements supported by those reference materials.

3.2.1 Sulfur in Coal

The method used most often for measuring the sulfur content in coal is ASTM method D 4239, Sulfur in the Analysis Sample of Coal and Coke Using High-Temperature Tube Furnace Combustion Methods. This method actually comprises three different methods:

- High-Temperature Combustion Method with Acid Base Titration Detection Procedures
- High-Temperature Combustion Method with Iodimetric Titration Detection Procedures
- High-Temperature Combustion Method with Infrared Absorption Detection Procedures

Among these three methods, the most common is the last. This method uses an infrared (IR) absorption detector to measure the amount of sulfur dioxide present in a sample of coal that is burned in a tube furnace. The method is based on the fact that sulfur dioxide absorbs IR energy at a precise wavelength within the IR spectrum. The amount of sulfur dioxide in the sample is proportional to the change in energy at the detector. Because this method is empirical, the apparatus must be calibrated.

The infrared detection system must be calibrated using SRMs, reference coals, or calibrating agents with known dry-basis sulfur values in the range of the samples to be analyzed. These SRMs, reference coals, or calibrating agents must have precision values of less than or equal to method repeatability.[3] They must be stable with respect to moisture and pulverized to pass 100 percent through a 0.250 mm (no. 60) USA Sieve.

Precision and Bias

ASTM reports the precision for the IR method as both the 2s method and the "d2s" measure described above. The precision intervals are reported in Table 3-1. These precision statements are valid for determining sulfur in the concentration range from 0.28 to 5.61 percent. The ASTM notes that this method has no bias if the instrument is properly calibrated against certified reference standards. This underscores the importance of unbiased SRMs in using this method.

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[3] NIST SRMs meet this criterion. For example, the NIST SRM for sulfur in coal, 2 percent (2683b), has a 95 percent confidence interval of ±0.041 percent, or 0.082 (NIST, 1997). At 2 percent sulfur, the repeatability interval for ASTM 4239 is about the same [0.02 + 0.03(2)] = 0.08 (ASTM, 1998).

Table 3-1. Characteristics of ASTM Testing Methods Used Most Often for Testing Sulfur in Fossil Fuels

The most frequently used methods for measuring sulfur in fossil fuels are instrumental methods; their accuracy depends on an unbiased calibrant.

ASTM Method Number	Title	Method Summary	Key Apparatus	SRM Usage	Bias	Repeatability (r) (2s)	Reproducibility (R) (d2s)
D 4239[a] (Method C)	Sulfur in the Analysis Sample of Coal and Coke Using High-Temperature Tube Furnace Combustion Methods	Uses IR absorption detector to measure the amount of IR absorption from a sample of coal that is burned in a tube furnace. Relationship between sulfur content and IR absorption is established by a calibration curve.	Commercially available sulfur analyzers with infrared detection systems	Used for calibration and periodic calibration verification	None when instrument is properly calibrated	$0.02 + 0.03\bar{x}$ $\bar{x}$ = average of two results	$0.03 + 0.09\bar{x}$ $\bar{x}$ = average of two results
D 2622	Sulfur in Petroleum Products by X-Ray Spectrometry	Uses an X-ray spectrograph to measure the intensity of sulfur radiation after the sample has been subjected to an X-ray beam. The relationship between radiation intensity and sulfur content is established by the calibration procedure.	X-ray spectrograph	Used for calibration quality control	No bias when appropriate corrections are applied	Sulfur Mass Fraction 0.0010 to 0.0049 0.0050 to 0.0149 0.0150 to 5.0000 r 0.60 * %S 0.20 * %S 0.05 * %S	R 0.60 * %S 0.40 * %S 0.16 * %S
D 5453	Determination of Total Sulfur in Light Hydrocarbons, Motor Fuels, and Oils by Ultraviolet Fluorescence	Uses an ultraviolet (UV) fluorescence detector to measure the amount of energy emitted from combustion gases after they have been exposed to UV light. Relationship between sulfur content and energy emission is established by a calibration curve.	UV fluorescence detector	Used for calibration quality control	Not reported[b]	$0.1867(\bar{x})^{(0.63)}$ $\bar{x}$ = average of two results	$0.2217(\bar{x})^{(0.92)}$ where $\bar{x}$ is the average of two results

[a] This ASTM method number covers three methods. This table discusses Method C, which uses infrared absorption detection procedures.

[b] ASTM reported that test results obtained on the SRM were within the repeatability of the test method.

Before coal can be analyzed for sulfur content, it must be sampled and prepared for analysis. Sampling and sample preparation are a significant source of uncertainty in coal sulfur content measurement. Two ASTM methods cover the procedures used for sampling coal:

- ASTM D 2234, Standard Practice for Collection of a Gross Sample of Coal
- ASTM D 2013, Standard Method of Preparing Coal Samples for Analysis

As described below, one way to improve the precision of the measurement of sulfur in fossil fuels is to increase the number of samples taken, analyze them separately, and report the average of the results. As described in ASTM D 2234, the control limits theory defines the relationship between the number of samples and precision. For example, to reduce the uncertainty by one-half (double the precision), four times as many gross samples must be taken. Similarly, to reduce errors to one-third (triple the precision), nine times as many gross samples must be taken. Increasing the number of increments in a gross sample can also increase the measurement's precision.

3.2.2 Sulfur in Petroleum Products

The methods used most often for measuring the sulfur content of petroleum products are ASTM D 2622, Sulfur in Petroleum Products by X-Ray Spectrometry, and ASTM D 5453, Determination of Total Sulfur in Light Hydrocarbons, Motor Fuels, and Oils by Ultraviolet (UV) Fluorescence.

D 2622 is required by EPA for verifying sulfur in diesel fuel. It is also required by the California Air Resources Board (CARB) for determining the sulfur content of high-sulfur fuels (exceeding 1,000 ppm). ASTM Method D 5453 is required by CARB to determine sulfur levels in low-sulfur fuels (1 to 8,000 ppm). D 5453 is much more sensitive than D 2622.

In ASTM D 2622, the sample is placed in an X-ray beam, and the intensity of the sulfur radiation is measured by an X-ray spectrograph. The calibration procedure establishes the relationship between radiation intensity and sulfur content. The measured intensity is then compared to the previously established calibration curve to obtain the concentration of sulfur.

The precision of this method is a function of the sulfur content of the sample. As shown in Table 3-1, the repeatability and reproducibility intervals, as a percentage of sulfur content, fall as the sulfur content grows.

In ASTM D 5453, a sample of a hydrocarbon is oxidized to SO_2. The sample combustion gases are exposed to ultraviolet light. A UV fluorescence detector is used to measure the light emitted by SO_2. The sulfur contained in the sample is a function of emitted light. The calibration procedure establishes the relationship between emitted light and sulfur content.

The precision of this method is shown in Table 3-1. As in the case of Method D 2622, the intervals become smaller (as a percentage of the concentration) as the concentration rises.

Both of these methods depend entirely on establishing a calibration curve, which, in turn, depends on a reliable calibration standard. If the calibration standard used to establish the calibration curve is biased, then the estimate of the sulfur content will be biased as well.

Petroleum products must also be sampled prior to analysis. Sampling of petroleum products is not as problematic as sampling of coal, because the product tends to be more homogeneous. ASTM Method D 4057 addresses practices for manual sampling of petroleum and petroleum products. Sampling crude petroleum and residual fuel oils is generally more difficult than sampling gasoline and distillate products because they are less homogeneous than gasoline and distillate products.

3.2.3 Reference and Sulfur Measurement

The instrumental methods used most often to measure the sulfur content of coal and petroleum products described above are based on the classic linear calibration model shown in Figure 3-3. They rely heavily on the use of standards and calibrants. As shown in the figure, if bias exists in the calibration standard used to calibrate the instrument this will translate to bias in the instrument's sulfur measurements.[4]

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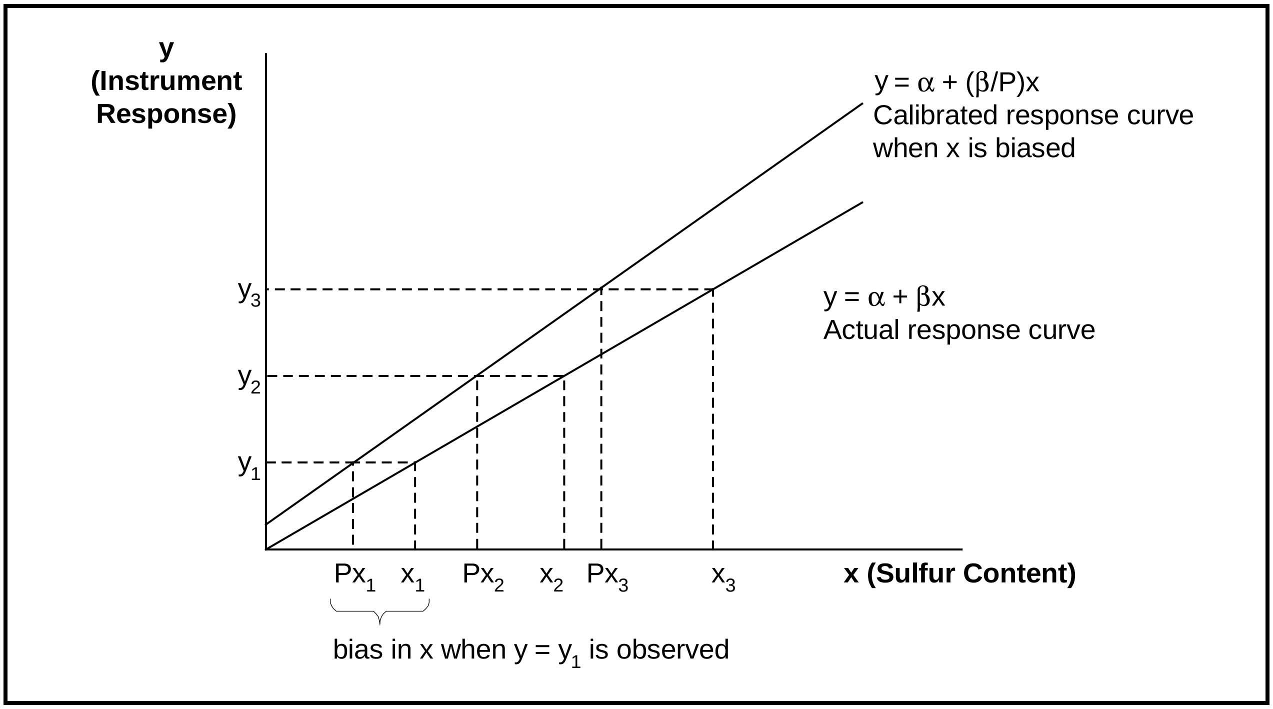
[4] Bias in the calibration standard is one potential counterfactual in the absence of NIST SRMs.

Figure 3-3. Classical Linear Calibration Model
If bias exists in the calibration standard this will lead to bias in the estimate of the slope of the curve and bias in estimates of the sulfur content.



Similarly, uncertainty about the certified value of a standard introduces uncertainty and additional bias to the measurements taken using the standard. The variance of the mean of n observations increases proportionately with the variance associated with the standard. These relationships are developed formally in Appendix A.

We can use these relationships to develop simulations of the impact of bias and variance in a reference material on the repeatability and reproducibility of ASTM methods. As noted above, bias in the certified value of a reference material translates into bias in the measurement of sulfur content. Thus, if NIST SRMs eliminate bias in calibration standards, they also remove bias from the measurement method.

3.3 IMPACT OF NIST SRMS ON THE MEASUREMENT OF SULFUR IN FOSSIL FUELS

NIST's SRM Program for sulfur in fossil fuels has improved the accuracy of the measurement of sulfur in fossil fuels. NIST's SRM development process is designed to provide a reference material that is unbiased and traceable to the System Internationale (SI) units. NIST's SRM program for sulfur in fossil fuels uses a definitive method, developed at NIST, that virtually eliminates bias and significantly reduces the uncertainty of the SRMs. Without the development of this method, sulfur measurement in industry would be subject to greater bias and uncertainty.

3.3.1 SRM Development Process

SRMs are developed in response to the measurement needs of industry and other NIST customers. Funding for research to support SRM development can come from NIST internal research funds, other government agencies, as well as from industry. The incremental costs associated with producing SRMs and maintaining the SRM program are recovered through sales. NIST must balance the application of its available resources versus the expressed need and projected impact in its SRM projects prioritization process, whether for new or renewal materials.

After identifying an SRM need, NIST conducts a careful analysis of the necessary properties of a useful reference material. Minimum specifications for a candidate SRM are drafted, and a material is obtained, usually from a naturally occurring source. Then measurements are made to evaluate the material's compliance with the specifications, and NIST begins the process of certifying the SRM.

SRM Certification: Basic Principles[5]

In certifying SRMs, the goal at NIST is to give a true value at a stated level of uncertainty for each property or constituent certified. Four major considerations are involved in certifying an SRM by NIST.

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[5] Much of this section is based on Taylor (1993).

Homogeneity. It is essential that every subportion of a given lot be the same within the overall uncertainty limits provided. This is necessary so that each user obtains a portion that agrees with the certified values. NIST conducts statistical assessments of the homogeneity of the material. The degree of homogeneity contributes to the uncertainty of the certified value.

Stability. If the material changes with time, it will eventually have true values that no longer agree with the certified values. NIST establishes the long-term stability of the material and includes any critical information concerning long-term storage or special stability requirements. In the case where this long-term stability has not been established, the certificate provides this information (e.g., "long-term [greater than one year] stability of this SRM has not been rigorously established. NIST will continue to monitor this material and any substantive change will be reported to purchasers"). Increasingly, SRMs are provided with expiration dates after which their certificate is not valid.

Handling Procedures. Special procedures, such as cold storage, drying, and other preparation may be necessary for the proper use of the SRM. In the case of some SRMs, segregation on standing is a potential problem. The certificate will instruct the user to shake, rotate, stir, or otherwise reconstitute the material. Failure to do so not only invalidates the present measurement but jeopardizes further measurement from the same container because of the disproportionate withdrawal of the contents.

Certified Values. The certificate must state the best possible level of accuracy for the certification. Sometimes this factor is stated as a tolerance interval; more often than not, it is simply given as an estimated uncertainty. NIST tries to provide conservatively stated uncertainties to allow for unknown systematic errors. The certified value is not expected to deviate from the true value by more than the uncertainty stated on the certificate. This uncertainty is more than a precision statement and includes the systematic error of the measurements, method imprecision, and material heterogeneity.

Certification: Hierarchy of Measurement Methods

Several techniques are especially helpful in the quest for certification accuracy. The quality of an SRM's assigned value is based on the existence and application of sound measurement principles and practices (May et al., 1999). Definitive, or primary, methods (methods of highest accuracy) are most closely linked to basic measurement units and thus reduce opportunities for error. Agreement of several independent laboratories using the same or different methods provides additional reason for confidence. Two approaches are used by NIST for fossil fuel SRM certification. In order of preference they are:

1. Single primary method approach: measurement by a definitive or primary method of known and demonstrated accuracy having essentially zero systematic errors. The measurements may then be confirmed using an additional technique.
2. Multiple independent method approach: measurement by two or more highly reliable independent critically evaluated methods, designated as reference methods having estimated inaccuracies (including systematic errors) that are small relative to the required certification accuracy.

In general, NIST uses approaches 1 or 2 to develop and certify SRMs such as sulfur content in fossil fuels. Below, we describe the hierarchy of measurement methods and how it is applied in the certification of an SRM.

Primary Methods. A primary method is a method of known and demonstrable accuracy. To understand the use of primary methods for SRM certification, one must also understand the SI system of units. The SI system of units includes the seven base units: mass, length, time, electric current, thermodynamic temperature, luminous intensity, and the amount of substance (i.e., the mole). Using the basic equations of physics, one can describe the approximately 50 derived units (e.g., volume, density, frequency, and viscosity) in terms of the base units. The derived units, together with the base units, form the basis for the other experimental measurement parameters that are normally determined in physics and chemistry laboratories (e.g., absorbance, nuclear cross-section, spectral intensity, pH). It is not always possible to relate the experimentally determined parameters to the basic units without using extensive approximations or inexact equations. These approximations may lead to large uncertainties in determining the experimental parameters by introducing systematic errors.

Although definitive methods are the most accurate methods available, they are not economical for general use because they require highly skilled personnel and specialized equipment and are time consuming.

A primary method is one in which all significant parameters have been related by a direct or solid chain of evidence to the base or derived units of the SI. These definitive methods have a valid and well-described theoretical foundation, have been experimentally evaluated so that reported results have negligible systematic errors, and have high levels of precision. Such methods with high reliability give true values and are the most accurate methods available to measure a given chemical property. They provide the fundamental basis for accuracy in chemical analysis. All potentially significant sources of error are evaluated explicitly for each application and investigated matrix (May et al., 1999).

Primary methods are generally uneconomical for general use. They usually require highly skilled personnel and are time consuming as well as expensive to perform. An example is the use of IDMS to determine the concentration of an element in a sample. In IDMS the concentration of unknown samples is related directly to the actual weights of spikes of isotopes or isotopically labeled compounds. In terms of accuracy, the IDMS technique is powerful because chemical manipulations are carried out on a direct weight basis, and the mass spectrometric determinations involve isotopic ratios rather than absolute isotope determinations, obviating the need for instrumental corrections. Thus, systematic errors are essentially eliminated. This technique automatically and directly results in determining experimental parameters in terms of base units of measurement. Examples of other definitive techniques are gravimetry and coulometry.

Once a value has been assigned to a reference material, that measurement is confirmed using an additional technique. Confirmation may be accomplished using one of the following three possibilities: a second NIST technique, interlaboratory testing, or determination of the certified constituents in other SRMs of similar matrix and constituent concentration (May et al., 1999).

Multitechnique Approach. Because primary methods are sometimes not available for use in certifying SRMs, NIST may sometimes use two or more independent critically evaluated methods for certification. Independent means that the basic principles used for the analysis must be entirely different. Reliable means that the method must have been successfully used in similar analytical situations (same concentration range, similar interferences) as that expected in certifying the SRM. The methods must be accompanied by a confident statement concerning the estimated systematic errors. To use a method, the estimated systematic errors must be small. The methods are chosen that have significantly different sources of error and variability. This approach is based on the rationale that the likelihood of two independent methods being biased by the same amount and in the same direction is small. A special kind of independent method is a reference method. This is a method of proven accuracy, based on testing versus a definitive method. Reference methods are generally arrived at by consensus.

SRM Certification

The actual testing of a material to be marketed as an SRM involves numerous stages of testing. The material must be tested to determine its homogeneity and stability. The certification analyses are conducted using critically evaluated methods. A statistical analysis is conducted to determine method imprecision and method biases, which are combined and reported as the uncertainty of the certified values.

The homogeneity of materials is usually relatively easy to establish once an adequate statistical sampling plan has been designed. Thus, analysts can use highly precise, rapid instrumental techniques such as x-ray fluorescence (XRF) or neutron activation analysis (NAA) to evaluate material variability without being concerned with the evaluation of systematic errors.

Materials with significant, but usable, levels of heterogeneity may be certified as a batch, in which case the statistical tolerance limits are given. A statement on the statistical tolerance limits includes the average value of all samples in the batch and limits within which most individual samples are expected to lie, with stated confidence. Because only a small number of samples will have been analyzed, the limits for a given percentage of samples cannot be stated with certainty. Rather, there is only a probability that the limits are valid. Thus, for example, it can be said with 95 percent confidence that these statistical tolerance limits cover the true values of 95 percent of the samples of the batch.

The final product of the certification of a NIST SRM is the SRM itself and the certificate of analysis accompanying it. The certificate presents the certified value—the best estimate of the value for a constituent or property of the SRM. This value is usually the arithmetic or weighted mean of the determinations made using definitive methods, independent methods, or from interlaboratory testing. A detailed discussion of alternative uncertainty measurements is provided in Taylor (1993).

3.3.2 History of NIST's SRM Program for Sulfur in Fossil Fuels

NIST's SRM program for sulfur in fossil fuels was motivated by anticipated needs due to the regulation of sulfur content in residual fuel oil. In 1967, NIST (then NBS) issued SRM 1621, Sulfur in Residual Fuel Oil, 1 %, and 1622, Sulfur in Residual Fuel Oil 2 %. The technical objective of the SRM work order for these two SRMs stated that

> The problem of air pollution from large industrial organization burning residual fuel oil containing sulfur has reached a point where legal limitations on the sulfur content of oils is a certainty. Out of these laws will arise considerable litigation, the outcome of which will depend on the ability to accurately analyze for the sulfur. The NBS sulfur in oil standard reference materials will supply a generally accepted, accurate standard against which the buyer and seller can check their oil for sulfur content as well as a standard for referee work in legal action.

The sulfur content for both of these SRMs was certified using a gravimetric method similar to ASTM D-129 (General Bomb Method). The relative uncertainty (95 percent confidence interval) of the certified value was about 2 percent of the certified value in the case of 1621, and about 0.5 percent of the certified value for the case of 1622. In the early 1970s, NIST added SRMs for other concentrations of residual fuel oil (SRM 1623) and also developed an SRM for distillate fuel oil (SRM 1624). Both of these were certified with the same gravimetric method used earlier, and the relative uncertainties were about 1.5 and 2 percent of the certified values, respectively.

Then NIST began the practice of using several independent methods to certify the standards. The independent methods usually included a gravimetric method, ion chromatography, microcoulometry, and X ray fluorescence. As shown in Table 3-2,

Table 3-2. Trends in Confidence Intervals for Certified Values of NIST SRMs
The introduction of the IDMS method has improved the accuracy of measurement methods for sulfur in fossil fuels.

SRM No. and Title/Certification Date	Certification Methods	Certified Value (CV)	Uncertainty	Uncertainty, Percentage of CV
1616: Sulfur in Kerosene				
1988	IDMS IC	0.0152	0.0002	1.32%
1995	IDMS	0.01462	0.00018	1.23%
1617: Sulfur in Kerosene				
1988	IDMS IC	0.169	0.004	2.37%
1995	IDMS	0.17307	0.00034	0.20%
1619: Sulfur in Residual Fuel Oil				
1981	GRAV IC XRF	0.719	0.007	0.97%
1991	IDMS	0.725	0.007	0.97%
1998	IDMS	0.696	0.0077	1.11%
1620: Sulfur in Residual Fuel Oil				
1979	GRAV IC	4.48	0.02	0.45%
1981	GRAV IC XRF	4.504	0.01	0.22%
1990	IDMS	4.22	0.013	0.31%
1621: Sulfur in Residual Fuel Oil ~1%				
1967	GRAV	1.05	0.02	1.90%
1980	GRAV IC	0.94	0.01	1.06%
1981	GRAV IC XRF	0.95	0.005	0.53%
1986	IDMS RR	1.04	0.015	1.44%
1991	IDMS	1.011	0.012	1.19%
1996	IDMS	0.948	0.0057	0.60%
1622 Sulfur in Residual Fuel Oil ~2%				
1967	GRAV	2.14	0.01	0.47%
1979	IC XRF	1.96	0.04	2.04%
1981	GRAV IC XRF	1.982	0.018	0.91%
1986	IC IDMS	2.012	0.025	1.24%
1991	IDMS	2.031	0.02	0.98%
1997	IDMS	2.1468	0.0041	0.19%
1623 Sulfur in Residual Fuel Oil				
1971	GRAV	0.268	0.004	1.49%
1981	GRAV IC XRF	0.24	0.003	1.25%
1990	IDMS	0.348	0.002	0.57%
1996	IDMS	0.3806	0.0024	0.63%
1624 Sulfur in Distillate Fuel Oil				
1971	GRAV	0.211	0.004	1.90%
1981	GRAV IC	0.141	0.002	1.42%
1990	IDMS IC	0.332	0.003	0.90%
1997	IDMS	0.397	0.004	1.01%

(continued)

Table 3-2. Trends in Confidence Intervals for Certified Values of NIST SRMs (continued)

SRM No. and Title/Certification Date	Certification Methods	Certified Value (CV)	Uncertainty	Uncertainty, Percentage of CV
1632 Trace Elements in Coal				
1975	Sulfur not Certified			
1978	Sulfur not Certified	1.64		
1998	GRAV IC XRF	1.89	0.06	3.17%
1633 Trace Elements in Coal Fly Ash				
1975	Sulfur not Certified			
1979	Sulfur not Certified			
1993	IDMS	0.2075	0.0011	0.53%
1635 Trace Elements in Coal (Subbituminous)				
1978	Sulfur not Certified			
1995	IDMS	0.33	0.03	9.09%
1819 Sulfur in Lubricated Base Oil				
1985(I)	MICRO XRF	299	8	2.68%
1985(II)	MICRO XRF	1,070	40	3.74%
1985(III)	MICRO XRF	2,865	70	2.44%
1985(IV)	MICRO XRF	6,030	130	2.16%
1985(V)	MICRO XRF	10,550	260	2.46%
1994(I)	IDMS	423.5	2.2	0.52%
1994(II)	IDMS	741.1	4.3	0.58%
1994(III)	IDMS	4,022	17	0.42%
1994(IV)	IDMS	4,689	21	0.45%
1994(V)	IDMS	6,135	23	0.37%
2294 Reformulated Gasoline				
1998	IDMS	$4.09\text{x}10^{-5}$	0.000001	2.44%
2295 Reformulated Gasoline				
1998	IDMS	0.000308	0.000002	0.65%
2296 Reformulated Gasoline				
1998	IDMS	0.00004	0.0000004	1.00%
2297 Reformulated Gasoline				
1998	IDMS	0.000304	0.0000015	0.49%
2682 Sulfur in Coal				
1982	GRAV IC TIMS	0.47	0.03	6.38%
1998	IDMS	0.486	0.006	1.23%
2683 Sulfur in Coal				
1982	IC GRAV TIMS	1.85	0.06	3.24%
1992	IDMS	1.89	0.03	1.59%
1997	IDMS	1.955	0.041	2.10%
2684 Sulfur in Coal				
1982	IC GRAV TIMS	3	0.13	4.33%
1992	IDMS	3.06	0.03	0.98%

(continued)

Table 3-2. Trends in Confidence Intervals for Certified Values of NIST SRMs (continued)

SRM No. and Title/Certification Date	Certification Methods	Certified Value (CV)	Uncertainty	Uncertainty, Percentage of CV
2685 Sulfur in Coal				
1982	IC GRAV TIMS	4.62	0.18	3.90%
1994	IDMS	4.73	0.052	1.10%
2690 Trace Elements in Coal Fly Ash				
1993	GRAV COLOR XRF	0.15	0.01	6.67%
2691 Trace Elements in Coal Fly Ash				
1993	GRAV COLOR XRF	0.83	0.05	6.02%
2692 Sulfur in Coal				
1988	GRAV IC TIMS	1.115	0.019	1.70%
1994	IDMS	1.184	0.036	3.04%
2717 Sulfur in Residual Fuel Oil				
1990	IDMS IC	3.022	0.024	0.79%
2724 Sulfur in Diesel Fuel Oil				
1992	IDMS	0.0425	0.0004	0.94%
1995	IDMS	0.04304	0.00037	0.86%
2775 Sulfur in Foundry Coke				
1999	IDMS	0.5816	0.0051	0.88%
2776 Sulfur in Furnace Coke				
1998	IDMS	0.825	0.016	1.94%

IDMS	Isotope Dilution Mass Spectrometry
IC	Ion Chromatography
GRAV	Gravimetry (ASTM D-120 for Petroleum; ASTM D-3177 for coal)
XRF	X-ray Fluorescence
RR	Round Robin
MICRO	Microcoulometry
COLOR	Colorimetry

[a] Uncertainty as reported on the SRM certificates. Two times the uncertainty value give the 95 percent confidence interval about the certified value.

NIST used several independent methods to certify SRMs from 1979 to 1981, including SRMs 1619, 1620 and 1620a, 1621a and 1621b, 1622a, 1623a, and 1624a.

In the early 1980s, NIST began developing an application of IDMS to the certification of sulfur in fossil fuels. P.J. Paulsen and W.R. Kelly developed a thermal ionization mass spectrometric method that utilizes iostope dilution, referred to as ID-TIMS. Their first paper describing the method appeared in *Analytical Chemistry* in 1984 (Paulsen and Kelly, 1984). For petroleum products, the first SRMs to be certified using IDMS were 1621C and 1622C in 1986 (although the application to coal came earlier, as explained below).

In general, NIST developed the certification statement using only the results from the IDMS, but NIST used other independent methods to confirm the results. Today, IDMS is considered a definitive method that virtually eliminates bias in the certified value and significantly reduces uncertainty.

NIST began certifying SRMs for sulfur in coal in the early 1980s with SRM 2682, 2683, 2684, and 2685. Although 1632 and 1635 were developed earlier, the sulfur levels for these SRMs were not certified until later. One of the earliest applications of the IDMS method for certifying sulfur in fossil fuels was in SRMs 2682, 2683, 2684, and 2685. At this early stage, IDMS was used in conjunction with other methods to confirm the certified value. IDMS is now used to certify virtually all SRMs for sulfur in fossil fuels.

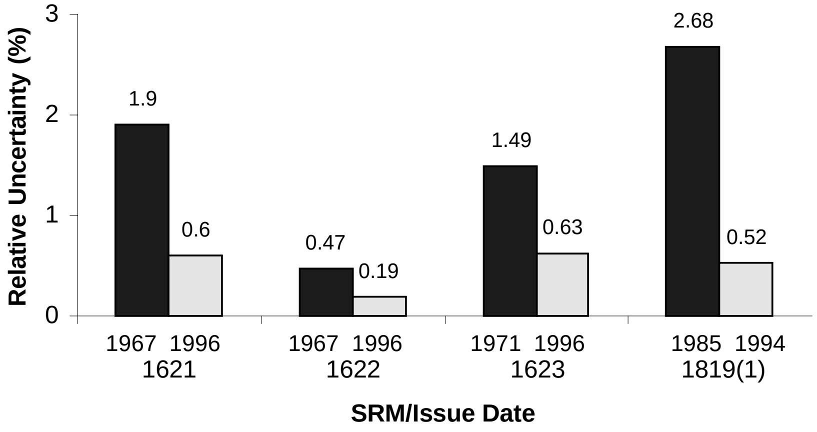
The application of IDMS has had a significant impact on the uncertainty associated with SRMs. Figure 3-4 compares the relative uncertainty for several SRMs over time. Part a shows relative uncertainties for SRMs for residual fuel oil and lubricating base oil. The first bar shows the relative uncertainty before the introduction of IDMS; the second shows the relative uncertainty of the most recently issued batches. For all petroleum products, the ratio of the relative uncertainty for the earliest SRMs to that of the most recent SRMs averages about 2.3.

A similar trend can be seen for the coal SRMs. The IDMS method has improved over the years. In 1982, the relative uncertainty of coal SRMs ranged from about 3 percent to about 6 percent. Today, the relative uncertainties range from 1 percent of the certified value to about 3 percent. For all coal SRMs the ratio of the relative uncertainty for the earliest SRMs to that of the most recent SRMs is about 1.6. Note, however, that these comparisons are more difficult for coal than for petroleum products because the heterogeneity of the material contributes a great deal to the SRM uncertainty.

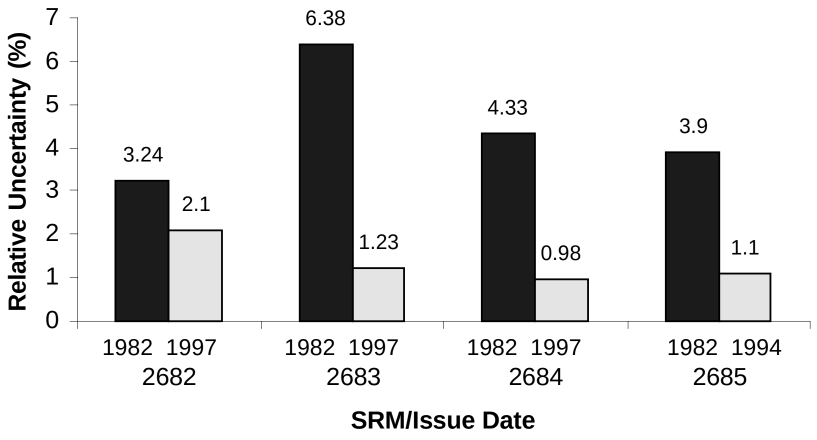
However, the uncertainty associated with NIST SRMs is only one component of the total uncertainty of the sulfur measurement methods. For example, in the analysis of coal, material heterogeneity is the primary source of uncertainty. Interviews with analysts at coal testing labs indicated that sample variability is

Figure 3-4. Impact of IDMS Method on the Relative Uncertainty of NIST SRMs for Sulfur in Fossil Fuels

The relative uncertainty of NIST SRMs decreased with the introduction of the IDMS method.



a) Petroleum Products



b) Coal

responsible for about 80 percent of the total uncertainty. Therefore, a reduction of the variability associated with the SRM has a small impact on the variability associated with the coal measurement itself.

For petroleum, sampling is not as important an issue. Interviews with chemists at petroleum refineries indicated that sampling error is responsible for about 33 percent of the total error. The uncertainty associated with NIST SRMs and instrument response account for a larger share of the total uncertainty of the sulfur measurement method. Therefore, we assumed that decreases in NIST SRMs' uncertainty may have a greater impact on sulfur testing in petroleum than in coal.

3.3.3 Counterfactual Scenarios

To analyze the impact of NIST's SRM program, we must develop a counterfactual scenario—that is, if NIST SRMs were not available, then what would be the state of the science for measuring sulfur in fossil fuels. For the counterfactual, we assume that, in the absence of NIST, the level of uncertainty associated with the measurement of sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the early 1980s.

We assume that, in the absence of NIST, the level of uncertainty associated with the measurement of sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the early 1980s.

Because of the complexity of the method and the skill and equipment required to apply IDMS, it is unlikely that any other laboratories developing CRMs would have pursued this method in the absence of NIST. This hypothesis was confirmed by our interviews with several CRM manufacturers who said that they typically do not engage in fundamental research targeted at new techniques for developing sulfur reference materials.

We assume that the impact associated with SRMs developed using the IDMS method began in 1986 and will continue at least through 2003. In 1986, NIST began selling SRMs developed using the IDSM method. However, not all benefits categories (described in Section 4) realized economic impacts beginning in 1986. For example, the decreased level of measurement uncertainty associated with SRMs using the IDMS method did not affect petroleum production until the mid-1990s when California began regulating the sulfur content of gasoline and diesel fuels.

4 Valuing Improved Sulfur Information

Information is "valuable" if it supports decisions that lead to improved economic outcomes. Information is then valued by comparing the outcomes obtained with and without the information (Preckel, Loehman, and Kaylen, 1987).

What is the value of improved information about the sulfur content of fossil fuels? Economic principles define information as "valuable" if it supports decisions that lead to improved economic outcomes. Information is then valued by comparing the outcomes obtained with and without the information (Preckel, Loehman, and Kaylen, 1987).

In this section, we apply this basic definition of the value of information to develop methods for valuing the benefits of NIST SRMs for sulfur in fossil fuels. First, we describe how sulfur information is used to support decisions in the fossil fuel industry. Second, we provide a set of hypotheses and a list of technical and economic metrics. Third, we discuss how the impact of NIST SRMs on measurement accuracy can be combined with primary and secondary data to test these hypotheses and value economic impacts. The last section describes how we collected the required data.

4.1 SULFUR INFORMATION AND ECONOMIC BEHAVIOR

Information about the sulfur content of fossil fuels is used in a number of industries to make decisions about product development, pricing, resource use, and production. More specifically, sulfur content measurements are used

- by the sulfur measurement industry to develop and produce sulfur measurement equipment, to prepare CRMs, and to conduct laboratory testing;

- by the fossil fuel supply chain to determine the appropriate price for fuels;
- by the fossil fuel supply chain for setting operating specifications for equipment to meet technical or regulatory criteria;
- by the fossil fuel supply chain for R&D aimed at developing new products and processes, including low-sulfur fuels and lubricants and desulfurization processes; and
- by the fossil fuel supply chain and the regulatory community (EPA and CARB) to verify compliance with environmental regulations.

Infratechnologies impact the economy by
- improving the efficiency of R&D,
- supporting the production process and enhancing product characteristics, and
- reducing transactions costs.

The potential impacts of these uses for sulfur information fall within the three categories of infratechnology impact discussed by Tassey (1997):

- **Infratechnologies improve the efficiency of R&D.** NIST SRMs for sulfur in fossil fuels may reduce the cost of developing new products and processes in the sulfur measurement industry and in the fossil fuel industry. They allow for the calibration and testing of sulfur measurement instruments, improve the quality of CRMs, and may improve the efficiency of research aimed at reducing the sulfur content of fossil fuels. SRMs allow for the replication and verification of research results.
- **Infratechnologies support the production process and can enhance product characteristics.** NIST SRMs support the production of the products and services of the sulfur measurement industry by providing quality control during the manufacturing and laboratory processes. For the petroleum refining and coal processing industries, NIST SRMs provide information that can improve their production processes, their products, and their environmental compliance. Improved sulfur information allows these companies to adjust the sulfur content of their inputs and outputs to more precisely meet technical and environmental specifications. For the electric power generation industry, higher-quality information can improve productive efficiency as well as reduce the risk of regulatory violations. For steel manufacturers, the quality of the steel is driven, in part, by the sulfur content of the coke that is used in this process; thus, more accurate information resulting from the use of NIST SRMs improves the quality and reliability of the product.

- **Infratechnologies reduce transactions costs.** Each market transaction involving a fossil fuel, from mining/drilling to combustion, depends on information about the sulfur content of that fuel. SRMs allow these measurements to be made accurately and enable comparability among the results, thus promoting efficient and low-cost transactions. SRMs also reduce transactions costs for consumers of instruments and CRMs. NIST traceability of these products assures customers of the quality of these measurement products.

Table 4-1 summarizes our observations about how NIST SRMs may support production stages for each of the three industry sectors that we discuss. We used this general characterization of the role of infratechnologies in the economy and the potential role of NIST SRMs for sulfur in fossil fuels to develop hypotheses about how NIST SRMs affect each of the affected market segments.

Table 4-1. Potential Impact of SRMs on Stages of Production in the Sulfur Measurement Supply Chain

NIST SRMS may affect several stages of production for each industry segment.

	Stage of Production		
Industry Sector	**R&D**	**Production**	**Market Transactions**
Sulfur Measurement Industry	✓	✓	
Fossil Fuel Processing	✓	✓	✓
Fossil Fuel Combustion		✓	✓

4.1.1 Use of SRMs and Sulfur Information to Improve R&D Efficiency

Both the sulfur measurement industry and the fossil fuel industry use NIST SRMs to develop new products and processes. NIST SRMs may support R&D by providing more accurate sulfur information. This support may decrease the cost and increase the efficiency of R&D.

Sulfur Measurement Industry

The sulfur measurement industry, including developers of CRMs, developers and manufacturers of sulfur measurement equipment, and independent labs, is prominent among the customers of NIST's SRMs for sulfur in fossil fuels. These organizations use NIST SRMs during the product development process to test alternative product designs and to develop new applications for their products. The availability of a standard for product testing may decrease the cost and increase the efficiency of product development.

Fossil Fuel Processing Industry

Petroleum and coal companies also use SRMs to conduct R&D to reduce the sulfur content of fuels and to improve sulfur testing methodologies. For example, fuel companies that would like better real-time information about the sulfur content of their products are developing in-line sulfur testing methods. NIST's SRMs improve the efficiency of these R&D processes by providing a standard for quality control and testing of new products and processes. However, these benefits are difficult to quantify.

4.1.2 Use of Sulfur SRMs to Support the Production Process

Improved sulfur content information can raise the quality of the products and services provided as well as make production processes more efficient.

Sulfur content information is used throughout the sulfur measurement industry and the fossil fuel supply chain to support production activities. The improved information can raise the quality of the products and services provided as well as make production processes more efficient.

Sulfur Measurement Industry

In addition to supporting the development of sulfur testing instruments and CRMs, SRMs support their production and the provision of sulfur testing services. NIST SRMs may improve the quality of these products and services because they support quality control. Improvements in the quality of these instruments, CRMs, and laboratory services in turn may increase their value to the customers of these companies because of the more accurate information they provide.

Fossil Fuel Processing Industry

The fossil fuel processing industry may use SRMs to support its fuel blending and fuel desulfurization activities. These companies blend coals and crudes of different characteristics, including sulfur content, to meet contract specifications regarding sulfur content. They may also conduct desulfurization processes for raw or final products to meet final sulfur specifications. If information about the sulfur content of the fuel is not accurate, the blend may be too high or too low in sulfur content. If it is too high in sulfur content, the buyer may not accept the shipment, or the seller may violate environmental regulations. If the sulfur content is below product specifications, the seller is essentially giving away product that could have been sold.

Accurate sulfur content information is important to fossil fuel producers because they conduct costly desulfurizaiton processes on raw or final products to meet contractual obligations.

Because of the uncertainty involved in measuring sulfur in fossil fuels, companies may include a “buffer” in their shipments. That is, they may ship fuel that measures lower in sulfur content than is specified in the contract. This buffer reduces the probability that the shipment will be rejected because it does not meet the terms of the contract. However, buffers are expensive because low-sulfur fuel commands a higher price than high-sulfur fuel and because desulfurization is expensive. Reducing the amount of the buffer may reduce the cost of meeting contract specifications.

Uncertainty about the sulfur content of finished petroleum products also affects the companies’ decisions regarding how to ensure environmental compliance of their finished petroleum products. Companies may use a “buffer” similar to that used in fuel blending and desulfurization processes described above to ensure compliance with sulfur content regulations.

Fossil Fuel Combustion Industry

Electricity generation equipment, especially environmental control equipment, is affected by the sulfur content of the coal that is used. Electrostatic precipitators remove particulates (fly ash) using electrically charged plates. The resistivity of the ash particles to the electric charges is adversely affected if the sulfur content becomes too high. Thus, if the sulfur content of the fuel is not known with certainty, technical specifications of this equipment may be set incorrectly. Process inefficiencies may result, increasing production costs.

Unknown sulfur content can also affect productivity by forcing the company to take action to prevent an environmental compliance violation. If the sulfur content of the coal is higher than expected, the company may be alerted to a potential violation by the information provided by the SRMs. The company may take action by reducing the fuel input in the boiler (reducing the productivity of the unit) or purchasing sulfur credits in emissions markets.

4.1.3 Use of Sulfur Information to Reduce Transactions Costs in the Purchase and Sale of Fuels and Other Products

SRMs can reduce transactions costs between buyers and sellers of fuels and other products by reducing the cost of acquiring the information (such as sulfur content) needed to set prices and finalize the transaction.

Recall that sulfur content normally is specified as part of a purchase contract. SRMs can reduce transactions costs between buyers and sellers of fuels and other products by reducing the cost of acquiring the information (such as sulfur content) needed to set prices and finalize the transaction. The primary characteristics of fossil fuel purchase contracts are explained below.

Sulfur Content Specifications

Coal purchase contracts generally specify a minimum and maximum sulfur content. Most long-term contracts will specify a range in which the coal's sulfur content must fall. The range is generally centered around a guaranteed value. The actual price paid for the shipment of coal may increase or decrease if the coal's actual sulfur content is above or below the guaranteed value. However, a buyer may reject a shipment if the sulfur content falls outside the specified range. Even then, the contract is not terminated if the seller makes reasonable assurances that it will remedy the situation. Similar negotiations occur for crude oil.

For finished petroleum products, the primary specification that must be met with respect to sulfur content is the sulfur limit imposed by either EPA or, in California, the CARB. The refineries test each batch of fuel produced. Pipeline companies may test the fuel before transporting it and prohibit the sulfur content from exceeding a set maximum limit related to the regulatory limit.

Pricing Based on Sulfur Content

A purchase contract for coal generally specifies a base price with price adjustments for differences in quality or changes in market price. A quality adjustment is almost always made for heat content (Btu/lb). A contract may have a quality adjustment for sulfur as long as the sulfur content is still within a specified range. For example, if the coal's sulfur content is lower than the guaranteed value, then the buyer pays a premium. The calculation of such a premium or penalty differs by contract.

Coal quality and price adjustments are typically applied to individual shipments, although some contracts will aggregate coal quality information on the basis of multiple shipments or for a given period. In the case of rail shipments, usually one composite sample applies for an individual shipment, and payment is based on that sample. In the case of truck deliveries, price and payment may be based on the average of samples taken from shipments over a period of time (all truck deliveries for a bimonthly or monthly basis). For barge deliveries, the price may apply to individual barge loads (1,500 tons each) or barge tows (nine barges or more).

The price of a crude oil shipment may be revised if the sulfur content varies from the guaranteed value. For refined petroleum, price is generally set for a specific type or grade of fuel, regardless of sulfur content, as long as it meets the (regulatory and performance) specifications. Although the price of a product might not change, lowering the sulfur content to meet a regulatory standard generally raises manufacturing costs.

Testing and Resolution of Disputes

Most coal contracts outline a general sampling procedure, which includes how many splits of each sample will be taken, who is responsible for sampling, and what procedure to follow if there is a dispute. Most specify that the testing facility must employ ASTM methods. The sampling plan and the testing site vary by contract. Usually they are not specified other than to mention that these must be carried out as agreed upon by the buyer and seller. Generally a sample is split into three portions. The seller (or the seller's designated laboratory) tests one portion, the buyer (or the buyer's designated laboratory) tests the other, and the third is kept in case of a dispute. In the event of a dispute, the third split is tested by an independent laboratory. Additional costs may be incurred by both parties to the transaction as they review the circumstances of the dispute and examine the data provided by the independent laboratory in comparison to their own test data.

For crude and refined petroleum, test methods are specified in regulations and contract and product specifications. The type (not brand) of equipment or instrumentation is usually described in the test method. Test methods include specific procedures for calibration. Most calibration procedures do not specify the use of NIST SRMs. SRMs or secondary standards based on SRMs can be used as part of a laboratory's quality control/quality assurance (QC/QA) program to check the test bias.

Intercompany contracts generally do not specify what happens in the case of a dispute regarding the sulfur content of petroleum products. In the case of EPA, an independent contractor collects and stores retained samples. EPA decides which 10 percent of the samples the independent laboratory must test. Results should agree with the refinery laboratory (within the reproducibility interval). In the case of a violation detected by EPA or CARB testing, a company could use its QC/QA data in defense. Test data on SRMs also are helpful in such cases.

4.2 HYPOTHESES

As described above, NIST SRMs affect each segment of the fossil fuel measurement industry and the fossil fuel supply chain. This section frames the discussion in Section 4.1 as a set of hypotheses about the impact of NIST SRMs on each sector. These hypotheses are summarized in Table 4-2.

4.2.1 Impact of SRMs on the Sulfur Measurement Industry

SRMs improve the quality of products and services by providing better quality control and a standard against which to calibrate instruments.

We expect that NIST SRMs have technical and economic impacts on the sulfur measurement industry (Table 4-2). SRMs reduce the cost of R&D by providing better information during the product development process. During the production process, SRMs improve the quality of products and services by providing better quality control and a standard against which to calibrate instruments. The technical impact is higher-quality equipment, more accurate CRMs, more accurate analytical results, and less product testing required. The hypothesized economic impact is consumers' higher valuation of products and services that provide greater accuracy of sulfur content information. To the extent that SRMs also reduce the need for product testing, they also may lower R&D costs.

Table 4-2. Hypotheses About the Impact of NIST SRMs
NIST SRMs may reduce R&D costs, increase the value of products, reduce fuel and operating costs, reduce regulatory penalties, and reduce sulfur emissions.

Beneficiaries/ Market Segment	Uses of NIST SRMs	Technical Impacts of Improved Information	Economic Impacts of Improved Information
Sulfur Measurement Industry			
Instrument Manufacturers	Calibrate equipment and control quality	Higher-quality equipment	Increased value to instrument users
	Verify product specifications during product development	Less product testing required during development	Lower R&D costs
Manufacturers of CRMs	Verify accuracy of CRMs Calibrate equipment	More accurate CRMs	Increased value to CRM users
	Verify product specifications during product development	Less product testing required during development	Lower R&D costs
Independent Laboratories	Calibrate instruments Control quality	More accurate analytical results	Increased value to users of services
Fossil Fuel Production and Combustion Industries			
Coal	Set prices and meet contract specifications	Fewer trade disputes over sulfur content	Lower transactions costs
	Determine level of desulfurization required prior to sales	Less uncertainty in coal blending process and desulfurization processes; less "buffer" to ensure limits are met	Lower costs for desulfurization; lower costs to meet contractual specifications
	Ensure and verify environmental compliance of products	Fewer environmental[a] compliance penalties	Reduction in number and dollar value of regulatory penalties
Petroleum Industry: Gasoline Diesel (distillate fuel oil) Kerosene Residual fuel oil Petroleum coke	Set prices and meet contract specifications	Fewer trade disputes over sulfur content	Lower transactions costs
	Determine level of desulfurization required prior to sales	Less uncertainty in fuel blending process and desulfurization processes; less "buffer" to ensure limits are met	Lower costs for desulfurization; lower costs to meet contractual specifications
	Ensure and verify environmental compliance of products	Fewer environmental[a] compliance penalties	Reduction in number and dollar value of regulatory penalties
	Verify product specifications during development of low-sulfur fuels and lubricants	Less product testing required	Reduced R&D costs

(continued)

Table 4-2. Hypotheses About the Impact of NIST SRMs (continued)

Beneficiaries/ Market Segment	Uses of NIST SRMs	Technical Impacts of Improved Information	Economic Impacts of Improved Information
Fossil Fuel Production and Combustion Industries (continued)			
Coke	Ensure sulfur content of coal and coke	Fewer trade disputes over sulfur content	Lower transactions costs
	Determine level of desulfurization required before and after coking	Less uncertainty in coal blending process and desulfurization processes; less "buffer" to ensure technical limits are met	Lower costs for desulfurization; may reduce fuel costs
	Determine settings for emissions control equipment	More efficiently operated emissions control equipment	Reduction in cost of controlling emissions
	Monitor and verify environmental compliance	Fewer environmental compliance violations	Reduction in number and dollar value of regulatory penalties
Electric Power Generation	Ensure sulfur content of purchased coal	Fewer trade disputes over sulfur content	Lower transactions costs
	Determine level of desulfurization required	Less uncertainty in coal blending process and desulfurization processes; less "buffer" to ensure technical limits are met	Lower costs for desulfurization; may reduce fuel costs
	Determine settings for emissions control equipment	More efficiently operated emissions control equipment	Reduction in generation cost
	Monitor and verify environmental compliance	Fewer environmental compliance violations	Reduction in number and dollar value of regulatory penalties
Steel	Ensure sulfur content of purchased coal and coke	Fewer trade disputes over sulfur content	Lower transactions costs
	Determine level of fuel desulfurization required	Less uncertainty in coal blending process and desulfurization processes; less "buffer" to ensure technical limits are met	Lower costs for desulfurization; may reduce fuel costs
	Determine level of post-production steel desulfurization required	Less uncertainty in steel desulfurization process	Lower costs for steel desulfurization
	Determine settings for emissions control equipment	More efficiently operated emissions control equipment	Reduction in production cost
	Monitor and verify environmental compliance	Fewer environmental compliance violations	Reduction in number and dollar value of regulatory penalties

(continued)

Table 4-2. Hypotheses About the Impact of NIST SRMs (continued)

Beneficiaries/ Market Segment	Uses of NIST SRMs	Technical Impacts of Improved Information	Economic Impacts of Improved Information
Regulatory Community and Environment			
Regulatory Community	Determine whether regulated community is in compliance with regulations	Less uncertainty and therefore more rigorous enforcement	Possible increased collection of regulatory penalties
		Lower emissions	Lower costs of environmental degradation

[a] Reductions in regulatory penalties are a transfer from regulators to companies but do not result in net benefits unless administrative costs also fall.

4.2.2 Impact on the Fossil Fuel Production and Combustion Industries

The fossil fuel production and combustion industries use sulfur information to inform a number of production and consumption decisions. Table 4-2 summarizes our hypotheses about the impact of this information on these industries. Many of the uses, technical impacts, and economic impacts across these industries are similar.

Setting Prices, Meeting Contract Specifications, and Ensuring Sulfur Content of Purchased Fuels

Accurate sulfur information can lead to fewer trade disputes over the sulfur content of the fuel, which can lower the transactions costs.

The coal, petroleum, and coke industries each are on the selling side (and in the case of coke, the buying side) of a fuel transaction. They use sulfur information to set prices and to meet their contract specifications. The purchasers of coal—the electric power and steel industries—use sulfur information to verify the sulfur content of what they have purchased. For each of these market participants, accurate sulfur information can lead to fewer trade disputes over the sulfur content of the fuel, which can lower the transactions costs.

Fuel Blending and Desulfurization

Sulfur information can also be used to determine (1) the extent to which fuels (including coal, crude oil, finished petroleum products, and coke) must be processed to remove sulfur, or (2) the proper degree of blending between high- and low-sulfur fuels. For suppliers of fuel, the information can lead to reductions in the cost of meeting the contractual specifications of fuel customers. To those processing fuel for their own use, it may decrease the cost of coal and petroleum processing.

Process Control

The electric power generation industry and the steel industry use sulfur content information to determine the proper fuel mix and to determine the settings required for emissions control. More accurate information can improve the efficiency of these processes.

Environmental Compliance

Sulfur information is also used by the regulated industries to monitor and verify their environmental compliance with sulfur content and sulfur emissions regulations. Improvements in their information about their compliance status may lead to fewer violations and regulatory penalties.

4.2.3 Impact on Regulatory Agencies and the Environment

Table 4-2 also summarizes our hypotheses regarding the impact of NIST SRMs on the regulatory agencies and the environment. EPA and CARB use sulfur SRMs to determine whether sulfur content regulations for gasoline and diesel fuel are being met. As the accuracy of sulfur content measurement improves, the enforcement of these regulations can also improve. For example, as stated earlier, CARB regulations for sulfur content of diesel fuel and gasoline state that enforcement will occur only if the sulfur content, as measured by CARB, is higher than the upper-bound reproducibility interval for the ASTM method specified in the regulation. Thus, as the reproducibility intervals of these methods narrow, the regulatory community can better enforce compliance with these regulations. This enforcement can lead to lower emissions, which reduces the economic damage to the environment.

4.3 VALUING ECONOMIC OUTCOMES

In the previous section, six main hypotheses were described:

H1: SRMs improve the quality of the products of the sulfur measurement industry. This quality improvement leads to a shift in demand and an increase in customers' willingness to pay (WTP) for these products and services.

H2: SRMs reduce the cost of R&D in the sulfur measurement industry and in the fuel industry by supporting accurate, reliable sulfur measurement.

H3: SRMs reduce the cost of fossil fuel transactions because measurements are accepted as reliable and fewer transactions are disputed because of measurement error.

H4: SRMs improve the efficiency of a number of production operations, including fuel blending, desulfurization, and equipment operations because the reliability of the measurement allows users to reduce the "buffer" they employ to ensure compliance with technical specifications.

H5: SRMs reduce the fines paid by industry due to environmental noncompliance because industry and the regulatory community have accurate and reliable sulfur content information.

H6: SRMs reduce the total amount of sulfur entering the environment by providing industry greater control over the sulfur content of its fuels and by allowing compliance officials greater authority in enforcing the regulatory limits.

These hypotheses suggest a number of economic impact measures for this study. Table 4-3 summarizes the technical and economic impacts developed and quantified through our interviews with members of the affected industries. Following the methodology illustrated in Figure 1-1, these technical and economic metrics are derived from the primary technical impact of NIST SRMs: improvement in the accuracy of sulfur content measurement.

This section describes how we valued the technical and economic impacts noted in Table 4-3. In particular, it focuses on quantifying six types of technical and economic impacts:

- benefits of improvements in product quality (H1);
- changes in R&D costs (H2);
- changes in transactions costs (H3);
- improvements in production efficiency (including changes in fuel costs, operating costs, and desulfurization costs) (H4);
- changes in regulatory penalties (H5); and
- benefits to the environment (H6).

Table 4-3. Technical and Economic Measures of the Impact of NIST SRMs
We used a variety of technical and economic impact measures to assess the impacts of NIST SRMs.

Hypothesis	Market Segment	Technical Impacts	Technical Impact Measure	Economic Impacts	Economic Impact Measure
H1: Improved Product Quality	Sulfur testing equipment CRMs Sulfur testing services	High-quality equipment, CRMs, and sulfur testing services	Change in repeatability intervals or confidence intervals	Higher prices commanded for products and services	Change in consumers' WTP
H2: Change in R&D Costs	Sulfur testing equipment CRMs	Less product testing required during development of equipment and CRMs	Change in product testing procedures (qualitative)	Lower R&D costs	Change in R&D costs
H3: Change in Transaction Costs	Coal, petroleum, coke, steel	Fewer trade disputes over sulfur content	Change in the number of trade disputes	Lower transactions costs	Change in total annual transactions costs
H4: Improved Production Efficiency	Coal, petroleum, coke, electric power, steel	More efficiency in coal blending, desulfurization, and processing	Change in the "buffer" used to ensure that technical and contractual specifications are met	Lower costs for desulfurization; lower raw fuel costs	Change in fuel costs; change in desulfurization costs
H5: Change in Regulatory Penalties	Electric power, steel	More efficiently operated emissions control equipment	Change in total amount of sulfur removed per Btu	Reduction in cost of emissions control equipment	Total change in annual operating cost
	Petroleum, electric power	Fewer environmental compliance violations	Change in the number of violations per year	Reduced regulatory penalties	Change in the total annual cost of regulatory penalties
H6: Benefits to Environment	Regulatory community	More rigorous enforcement	Number of enforcement actions per violation	Collection of regulatory penalties	Total annual collection of regulatory penalties
	Environment	Lower emissions	Total annual emissions of sulfur	Cost of environmental degradation from sulfur	Change in the cost of environmental degradation from sulfur

4.3.1 Benefits of Improvements in Product Quality (H1)

The value of an improvement in the quality of a good or service can be measured by a change in the sum of producers' and consumers' surplus. Consumers' surplus is a measure of the net benefit received by consumers from the purchase of a good or service. It is the difference between what the good or service is worth to the buyer and what they actually pay for it (the price). Producers' surplus is the difference between what producers receive for a good (the price) and what it costs to produce it. The total welfare created by a market transaction is equal to the sum of producers' and consumers' surplus.

To simplify our analysis, we assumed that marginal cost is constant and equals price. This implies that producers' surplus is zero; all net benefits created by a market transaction accrue to consumers. This assumption does not affect our estimate of the total benefits of improvements in product quality; however, it does mean that we cannot describe the distribution of these benefits among buyers and sellers.

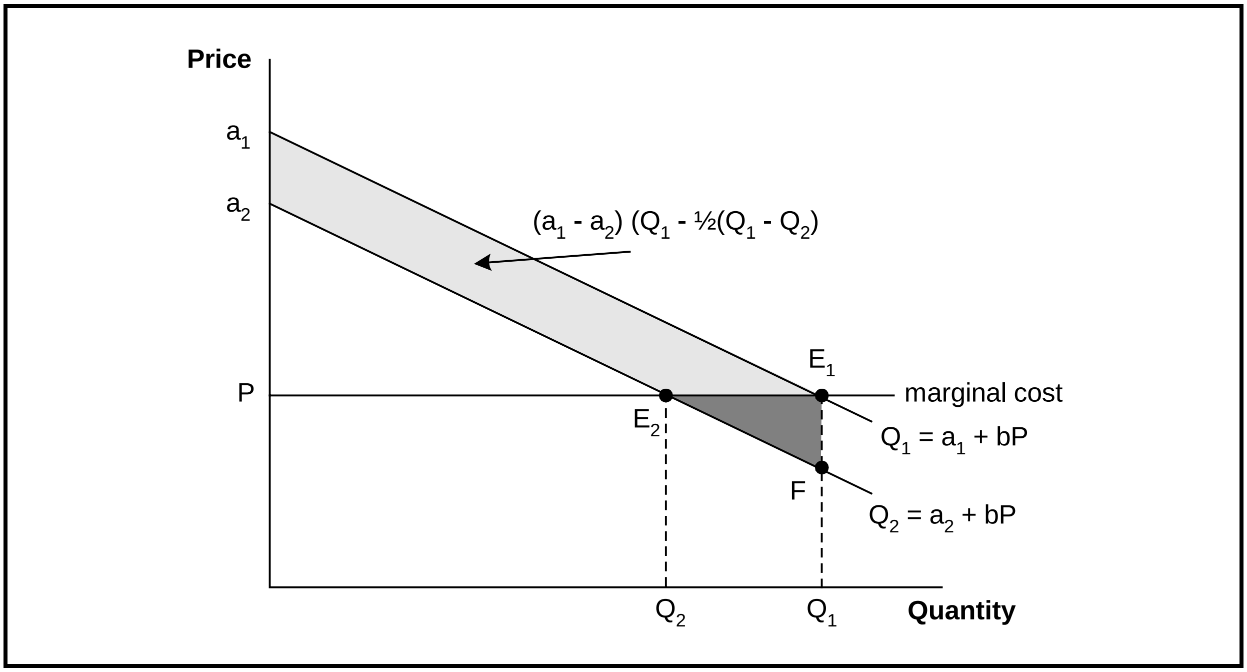
The value of a good or service to any given consumer can be quantified by his or her WTP for this good or service. WTP is an observable measure of utility that is typically used in benefit-cost analyses. It is a measure of the maximum dollar amount the individual would be willing to pay for the welfare improvement we would expect from the quality changes. Although WTP is not a perfect surrogate for utility changes, the consensus among economists is that WTP does provide the best available utility surrogate (Haddix et al., 1996; Sloan, 1995; Tolley, Kenkel, and Fabian, 1994).

In some cases, WTP is revealed in markets. When an individual purchases a commodity in a market, the monetary sacrifice is the price of the commodity. In such cases, price is the appropriate WTP value of the welfare change associated with a one-unit increase in the individual's consumption rate of the commodity.

A demand curve is a representation of the relationship between quantity and consumers' WTP. Figure 4-1 demonstrates this relationship and how it might be affected by changes in product quality. Assume the current (with-NIST) demand curve for a CRM, for example, is

Figure 4-1. Change in Consumers' Surplus for Products and Services Produced with NIST SRMs

In the absence of NIST SRMs, demand shifts downward and consumers' surplus falls by the area $a_1E_1E_2a_2$.



$$Q_1 = a_1 + bP,$$

where

Q is the quantity demanded,

P is price,

a is the intercept,

b is the inverse of the slope, and

subscripts indicate the with-NIST (Scenario 1) or without-NIST (Scenario 2) demand.

Marginal cost is constant and is therefore equal to the market price. The net benefits to all consumers who purchase the CRM are equal to area PE_1a_1. Now suppose that without the NIST SRM this demand curve would shift downward because the quality of the CRM (e.g., accuracy of its certified value) would decline. The new (without-NIST) demand curve would be

$$Q_2 = a_2 + bP.$$

We assume that the elasticity of demand does not change. Thus, as shown in Figure 4-1, the change in quality causes a parallel shift in the demand curve. Consumers' per-unit WTP for this product falls by the amount ($a_1 - a_2$). This decline leads to a reduction in the equilibrium quantity demanded from Q_1 to Q_2 and a reduction in consumers' surplus. In this case, the consumers' surplus falls to area PE_2a_2. The loss in consumers' surplus is equal to $a_1E_1a_2E_2$. This is the appropriate measure of the change in welfare due to the use of NIST SRMs.

The change in consumers' surplus (CS), using the simplifying assumptions stated earlier (linear demand, constant marginal cost), can be expressed as

$$\Delta\ CS = (a_1 - a_2) * [Q_1 - \tfrac{1}{2}(Q_1 - Q_2)]$$

To implement our methodology for estimating the benefit of an improvement in the quality of goods and services due to NIST SRMs, we needed to collect variables for each good and service that is manufactured with the assistance of NIST SRMs for sulfur in fossil fuels. These variables are

- annual quantities sold,
- prices, and
- estimates of change in consumers' in WTP for each product.

Table 4-2 provides an example of the type of data we collected to implement the measurement plan. As shown in Appendix B, we designed survey questions that elicit this information. Note that we assumed that the manufacturers of these products can estimate the change in their customers' WTP. Ideally, we would ask the customers for this information; however, this population is too large and difficult to identify to make this a reasonable task within the resources allowed for this study.

4.3.2 Changes in R&D Costs (H2)

We hypothesized that the manufacturers of instruments and CRMs, as well as fuel companies, benefit from accuracy in the measurement of sulfur via reductions in the cost of R&D. To quantify these changes, we collected and analyzed the following information:

- total R&D budget for industrial sector (B);
- percentage of R&D budget allocated to sulfur-related research (D);
- percentage of R&D costs consumed by measurement and testing of sulfur content (T); and
- potential percentage increase in R&D costs due to unavailability of NIST SRMs for sulfur in fossil fuels (M).

The decrease in R&D cost to industry is then

$$\Delta C = B * D * T * M.$$

4.3.3 Changes in Transactions Costs (H3)

We hypothesized that increases in the precision of the measurement of sulfur in fossil fuels decrease the transactions costs for buyers and sellers of fossil fuels. To quantify the extent of these changes, we need to know

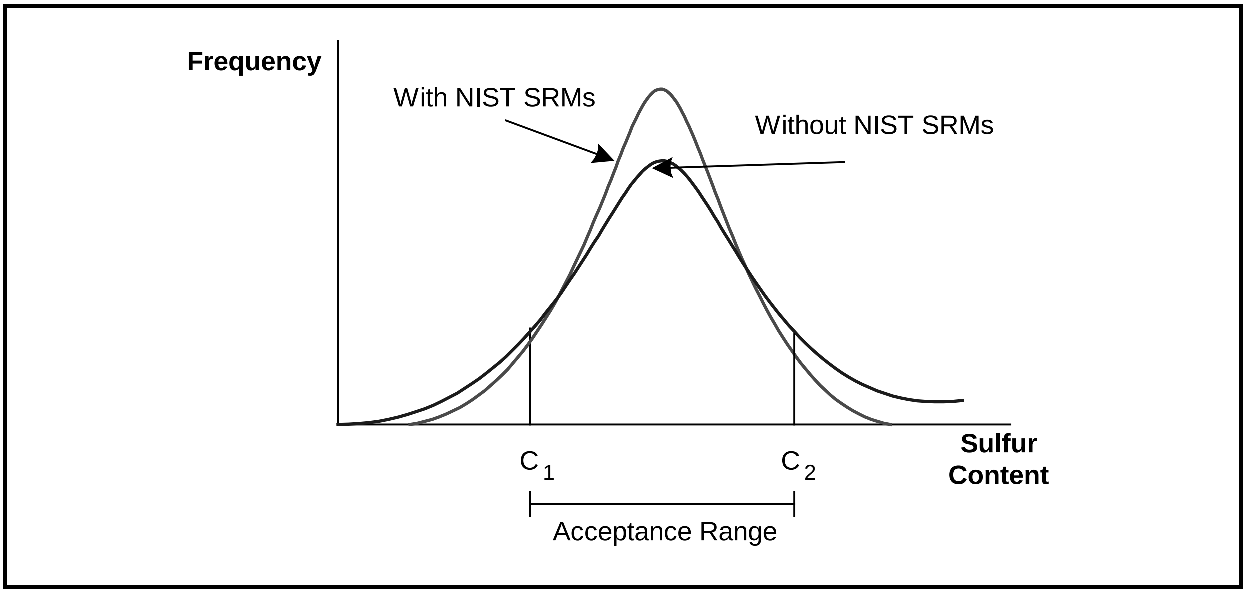
- the number of fossil fuel transactions that take place each year;
- the number of transactions that currently involve some type of dispute over the sulfur content of the fuel;
- the impact of NIST SRMs on the number of transactions in dispute; and
- the cost of resolving a dispute.

From our analysis of the impact of SRMs on the repeatability of sulfur measurements, we estimated the change in the number of disputes. This estimate depends on the degree to which the SRM improves the precision of the measurement of sulfur in fossil fuels. As this precision increases, fewer shipments are disputed because of measurement error. Our approach is illustrated in Figure 4-2.

As previously described, many fuel purchase contracts specify a sulfur content and a range within which the shipment will be accepted. Assume that the acceptance range is C_1 to C_2—that is, the purchaser of the fuel will accept the shipment as long as the estimated sulfur content lies [above C_1 or] below C_2. For simplicity, assume that this acceptance range is equal to the 95 percent confidence interval for the measurement of sulfur in fossil fuels, and that a NIST SRM is used for calibration and/or quality control. These assumptions imply that if one measurement is within the acceptance range, a second measurement will be

Figure 4-2. Impact of SRMs on Disputes due to Measurement Error

Given a fixed acceptance range, improved measurement precision decreases the probability of rejection.



below C_1 or above C_2 5 percent of the time because of measurement error.

If we assume that sulfur measurements (x) are distributed normally with a mean of $\bar{x}$ and a standard error of s, then the following relationships apply:

With-NIST SRMs:[1]

$C_1 = \bar{x} - 1.96\sqrt{2}\, s$

$C_2 = \bar{x} + 1.96\sqrt{2}\, s$

Prob $x < C_1 = 0.025$ (because 0.975 is the area under the cumulative normal curve at 1.96)

Prob $x > C_2 = 0.025$

Total probability of rejection due to measurement error = 0.05

In the absence of NIST SRMs, we know that the confidence interval widens because the standard error of the distribution, s′, is larger. For petroleum products, s′—the value of the standard error without NIST—is about 2.3 times what it is with NIST SRMs. For coal, the

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[1] The difference "two" standard deviation limit (d2s) is used to calculate the acceptance interval (described in Section 3.1.2) because disputes typically involve the comparison of *pairs* of test results—one by the seller and one by the purchaser of the fossil fuel.

without-NIST s is about 1.6 times what it is with NIST SRMs.[2] Taking coal as an example, the following relationships hold:

$$s = s'/1.6$$

$$C_1 = \bar{x} - \left(\frac{1.96\sqrt{2}s'}{1.6}\right) = \bar{x} - 1.255\sqrt{2}\ s$$

Prob $x < C_1 = 1 - 0.8897$ (area under the cumulative normal curve at 1.225) = 0.0951

Prob $x > C_2 = 0.1103$

Total probability of rejection due to measurement error is about 0.22

Thus, the probability that a shipment will be disputed changes from 0.05 in the with-NIST case to about 0.22 in the without-NIST case. If the total number of transactions per year sold on the basis of sulfur content is equal to 1 million, the number of transactions in dispute climbs from 50,000 in the with-NIST case to 220,000 in the without-NIST case. (This is an extreme example. The real numbers are much smaller.)

To implement this analysis, we collected information on the number of transactions that specify sulfur content, the percentage that currently are disputed, and the cost of resolving a dispute. Information about the impact of NIST SRMs on the distribution of sulfur measurements was determined as described in Section 3.

4.3.4 Improvements in Production Efficiency (H4)

We hypothesize that by improving the quality of the measurement of sulfur in fossil fuels NIST SRMs assist the coal, petroleum, steel, and electric utility industries in improving the productivity of many of their operations. These operations include fuel blending, desulfurization, and operation of equipment. In this section, we describe how we quantified and valued these changes in productivity.

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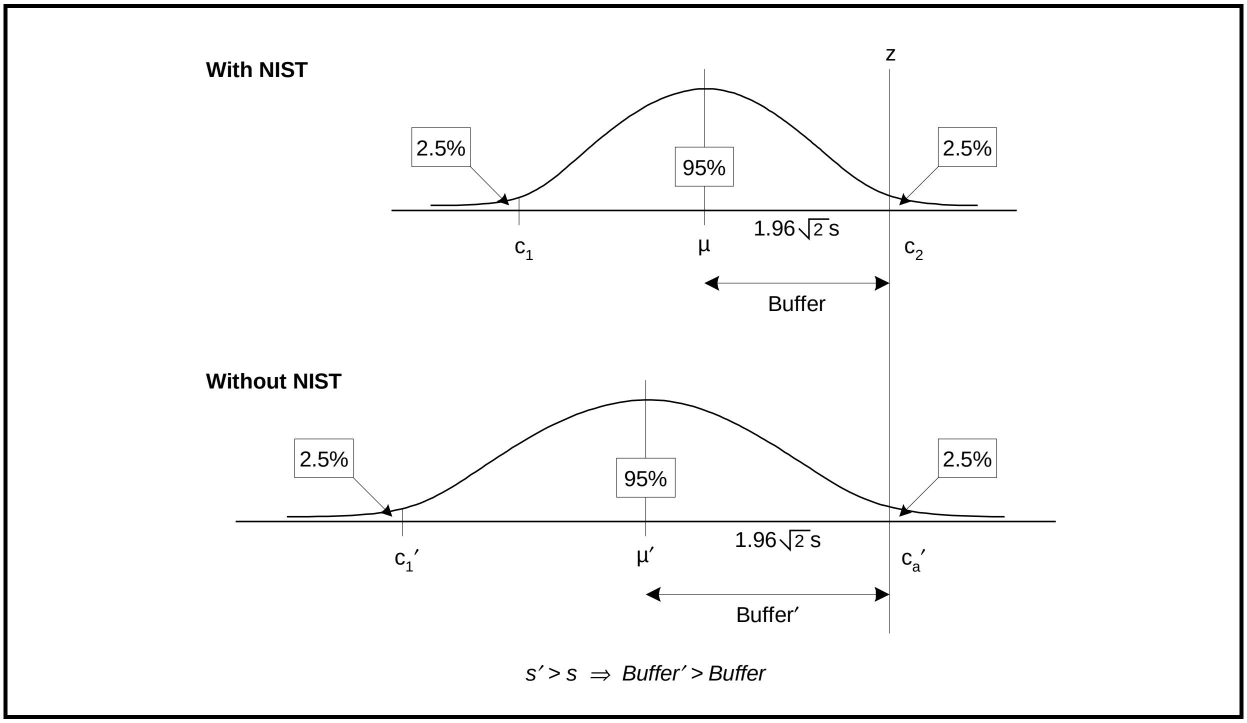
[2] These factors represent the average ratio of SRM standard errors before and after introducing the IDMS methodology.

Quantifying the Economic Benefits of Improvements in Efficiency

As described in Section 3.1.2, lack of perfect information about the sulfur content of fuel leads to inefficiency in the production, processing, and combustion of fossil fuels where sulfur content is a technical or regulatory factor. The primary factor affecting productivity is companies' use of a "buffer" to ensure that they have met the specification. Figure 4-3 illustrates this concept.

Figure 4-3. Impact of NIST SRMs on Buffers
Improved measurement precision may decrease the size of buffers used to ensure that technical specifications are met.



Suppose the critical level for the sulfur content of a batch of fossil fuel is equal to z, and that there is a penalty associated with going over z. For this reason, sellers may intentionally target a sulfur content that is less than z to provide some degree of assurance that when the buyer (or regulator) measures the sulfur content it will be below cutoff level. Let C_1 to C_2 be the 95 percent reproducibility interval of the measurement method, assuming that NIST SRMs are available. Thus, the seller is 95 percent certain that if its measurement is μ, a second measurement will lie within that interval.

The following relationships hold:

$$C_1 = \mu - 1.96\sqrt{2}\ s$$

$$z = C_2 = \mu + 1.96\sqrt{2}\ s$$

For example, suppose the critical sulfur level for diesel fuel is 500 ppm and the oil company wants to be 95 percent certain that the fuel will test at or below 500 ppm. If the reproducability interval is equal to 50 ppm, then the oil company would set the target value at 475 ppm to be 95 percent certain that the fuel would test at or below 500 ppm. The buffer would be equal to 25 ppm, about half of the reproducability interval.

Now consider the impact of a wider interval (e.g., the impact of a wider interval due to the absence of a NIST SRM). For petroleum products, that standard error in the absence of NIST SRMs is about 2.3 times the size it is, given the availability of NIST SRMs. This implies the buffer increases to approximately 57 ppm and the new target value (μ') is equal to about 443 ppm.[3]

To value the impact of the change in the buffer, we must consider the relative cost of low-sulfur versus high-sulfur fuels. For petroleum products, we used the unit desulfurization costs of gasoline and diesel fuel ($0.0001 per gallon to remove 1 ppm of sulfur—see Section 4). For coal, we conducted a similar analysis; the value of reducing the sulfur buffer is based on the unit cost of cleaning and blending coal to remove sulfur (approximately $0.03 per ton per 0.01 percent sulfur reduction—see Section 4).

To complete the analysis, we multiplied the per-unit savings due to the reduction of the buffer by the annual quantity of fuel subject to each type of constraint. For example, we needed to know the annual quantity of diesel fuels subject to the 500-ppm sulfur limit imposed by EPA, the quantity of gasoline subject to the sulfur limits, and the quantity of fuels subject to sulfur limits in purchase contracts and for technical operating criteria.

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[3] We have simplified this example. Actually, the reproducibility interval function changes with changes in the mean sulfur concentration.

4.3.5 Changes in Regulatory Penalties (H5)

In addition to causing changes in the efficiency of production, improvements in the measurement of sulfur content may reduce the incidence and quantity of penalties imposed by the regulatory community. As a result, NIST SRMs may reduce the expected value of regulatory penalties for industry.

Suppose that the penalty for being over the limit on diesel fuel can be expressed as follows:

$$\text{Fine} = G * (x - 500) * F$$

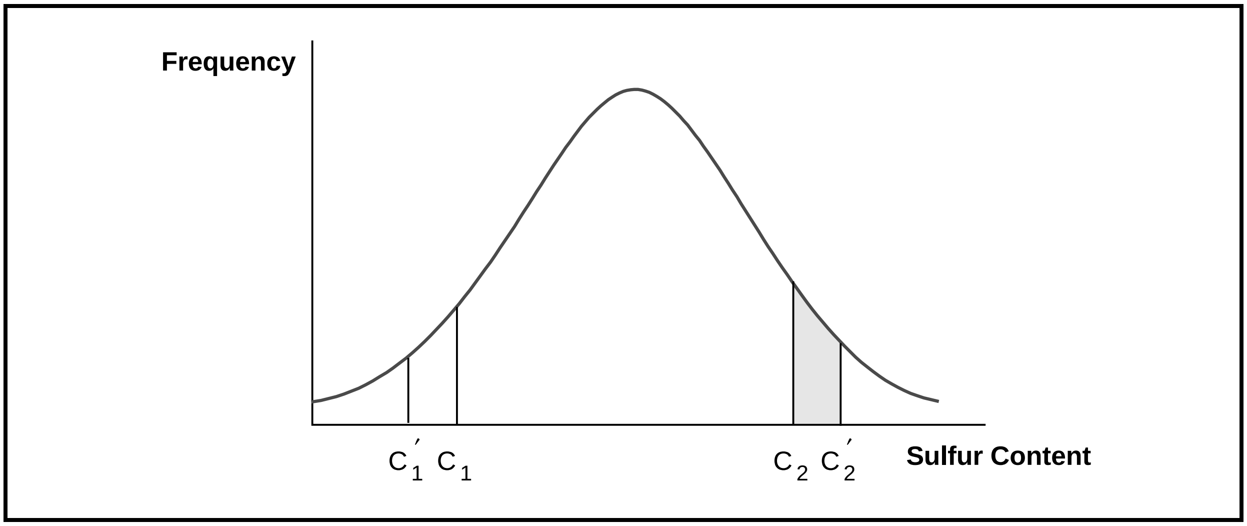
where G is the number of gallons in the batch; F represents the per-gallon, per-ppm fine associated with overshooting the sulfur limit; x is the sulfur value as measured by the regulatory authorities; and 500 is the regulatory limit in ppm. The expected value of the fine is a function of the standard deviation associated with the measurement, x. Because NIST SRMs reduce the standard deviation of this measurement distribution, they decrease the expected total loss associated with the probability of being over the limit.

4.3.6 Benefits to the Environment (H6)

As the probability of exceeding regulatory limits for sulfur in fossil fuels falls, emissions of sulfur to the environment may also fall. Thus, improving the measurement of sulfur empowers regulated industries not only to avoid regulatory penalties, but also to avoid emitting sulfur to the environment. In addition, some regulations specify that compliance actions can only be taken if the test results of the regulatory authority exceed the reproducibility interval. Thus, achieving a narrower reproducibility interval allows for improved compliance with the regulation.

Figure 4-4 demonstrates the impact of narrowing the reproducibility interval on regulatory compliance. Suppose the reproducibility interval with NIST SRMs is C_1 to C_2. Any company whose products test in excess of C_2 is subject to regulatory enforcement and the batch cannot be sold. However, suppose the reproducibility interval in the absence of NIST SRMs is C_1' to C_2'. This means that the regulatory agency cannot take action unless the sulfur tests higher than C_2'. This implies that, in the absence of NIST SRMs,

Figure 4-4. Impact of NIST SRMs on Regulatory Compliance Activities
NIST SRMs may improve testing methods to prevent noncompliant fuels from entering commerce.



batches of fuel testing at between C_2 and C_2' would be allowed to enter commerce. To determine the impact of this change on the environment, we gathered information on the

- quantity of fuel currently testing outside the reproducibility interval (greater than C_2),
- ranges of sulfur values for batches testing outside the limits, and
- changes in reproducibility intervals from the simulation exercises described in Section 3.

This information allowed us to estimate an expected decrease in sulfur emissions:

$$\int_{C_2}^{C_2'} f(x)\,(x - C_2)\,dx$$

where x is the tested value of the sulfur content.

4.4 DATA COLLECTION

We hypothesized that NIST SRMs provide a variety of benefits to industries that use SRMs and sulfur measurement products and services. This section describes our procedures for collecting the data required to test these hypotheses. First, we summarize the data requirements from each industry sector. Then we discuss how we chose the sample of companies from among the many companies likely to be affected by NIST SRMs. Finally, we discuss our data collection procedures, including the procedures we used to pretest the instruments, contact participants, and record their responses.

4.4.1 Data Requirements

A variety of data are needed to test the hypotheses we developed earlier in this chapter. We also developed technical and economic impact measures and described the data that would be needed to construct each measure. Table 4-4 summarizes these data requirements.

The final column in Table 4-4 indicates the source of the data. We collected items marked "secondary" from publicly available secondary data sources. Many of these data items were available from EPA, CARB, the American Petroleum Institute, and the Electric Power Research Institute. When possible, we verified these data during the interviews. For data elements for which the source is marked "primary," we collected these data directly from interview participants. Appendix B contains the questionnaire used to guide the interviews.

4.4.2 Sample Selection

We interviewed several members of each of the affected industries. The interview contact list was developed using information and contacts provided by our consultants, industry trade associations, the SRM sales database, and the ASTM online directory of testing laboratories. Table 4-5 shows the number of interviews conducted by industry segment. Although we spoke with many of our respondents on multiple occasions over the course of the study, each respondent was counted as one interview. Occasionally, it was necessary to conduct interviews with multiple contacts within one company, because of the range of activities conducted in different divisions of larger companies.

Table 4-4. Data Elements Required to Populate the Analytical Model
The evidence required to support our six hypotheses will be collected from both primary and secondary sources.

Hypothesis	Affected Industries	Data Elements	Source
H1	Sulfur measurement industry: ➤ CRM manufacturers ➤ Sulfur testing equipment manufacturers ➤ Sulfur testing laboratories	Product quantities	Secondary
		Product prices	Secondary
		Quality change	Primary
		Customer WTP for quality change	Primary
H2	➤ Sulfur measurement industry ➤ Fossil fuel industry, especially petroleum companies	Industry R&D budget	Secondary
		Percentage of R&D allocated to sulfur-related research	Primary
		Percentage of R&D costs consumed by measurement and testing of sulfur content	Primary
		Potential percentage increase in R&D costs due to unavailability of NIST SRMs for sulfur in fossil fuels	Primary
H3	➤ Fossil fuel extraction, processing, and transportation ➤ Fossil fuel generation	Annual number of transactions	Secondary
		Percentage specifying sulfur content	Primary
		Percentage of transactions currently disputed	Primary
		Cost of resolving a dispute	Primary
H4	➤ Fossil fuel extraction, processing, and transportation ➤ Fossil fuel generation	Annual quantity of fuel subject to sulfur specification	Secondary/ primary
		Penalties for overshooting specification	Secondary/ primary
		Cost of undershooting	Secondary/ primary
		Use of buffers	Primary
H5	➤ Fossil fuel extraction, processing, and transportation, especially petroleum companies ➤ Fossil fuel combustion	Fine structure of regulation	Secondary/ primary
		Quantity of fuel subject to regulation	Secondary
		Annual quantity of fuel exceeding regulatory limits	Primary
		Annual quantity of fines assessed	Secondary
H6	➤ Regulatory community (EPA, CARB)	Compliance structure of regulations	Secondary/ primary
		Quantity of fuel currently testing outside compliance guidelines	Secondary/ primary
		Average sulfur values for noncompliant fuels	Primary
		Economic damages associated with SO_2 emissions	Secondary

Table 4-5. Number of Interviews by Industry Segment
We interviewed several members of each affected industry segment.

Industry	Number of Interviews	Number of Companies[a]	Percentage of Industry Revenue
Sulfur Measurement Industry			
Instrument manufacturers	4	4	12
CRM manufacturers	5	4	44
Independent testing laboratories	3	2	14
Fossil Fuel Extraction, Processing, and Transportation Industry			
Coal companies	5	4	10
Coke companies	0	0	0
Petroleum companies	5	3	18
Fossil Fuel Combustion Industry			
Electricity generation firms	6	3	7
Steel companies	3	2	12
Regulatory Agencies	5	1	
Total Interviews	38	24	

[a] For several larger companies, we spoke with two or more divisions.

The interviews were conducted in two stages: scoping interviews and technical interviews. During the scoping interviews, we learned about sulfur-content testing, methods and practices, and the importance of accurate sulfur-content information. We then used this information to develop and refine the questionnaire for the technical interviews. During the technical interviews, respondents were asked about sulfur testing and SRMs, their impressions of the impact of SRMs, and their use of the sulfur-content information.

Sulfur Measurement Industry

We interviewed companies from each segment of the sulfur measurement industry:

- instrument manufacturers,
- manufacturers of CRMs, and
- independent testing laboratories.

The companies interviewed for each of these segments represented 12, 44, and 14 percent of total industry revenue, respectively. Table 4-6 lists the companies and organizations we interviewed.

Table 4-6. Companies Interviewed
Twenty-four companies, associations, and agencies participated in this study.

American Iron & Steel Institute
Antek Instruments
Asoma Instruments
Bethlehem Steel
California Air Resources Board
Carolina Power & Light
Chevron Research & Technology
Commercial Testing & Engineering
Conoco
Duke Energy
Electric Power Research Institute
Interprovincial Pipeline
Leco Corporation
MAPCO Coal
Mobil Research & Development
National Mining Association
NSI Solutions
Oxford Instruments
RAG American
SPEX Certiprep
Standard Laboratories
Tennessee Valley Authority
Vanguard Solutions
VHG Labs

We spoke with four instrument manufacturers. Several criteria were used in selecting instrument manufacturers to interview. First, we targeted companies whose sole line of business was analytical equipment. Second, these companies produce well-known instruments that are used to conduct tests for sulfur in fossil fuels. Many of our other respondents used the instruments these companies produced in their laboratories. Finally, we included both small and large companies in the interviews to investigate if instrument development and manufacturing varies by company size.

We spoke with four CRM companies. Using sales data supplied by NIST, we generated a list of eight companies whose primary line of business is developing reference materials traceable to NIST SRMs. From this list we selected two small and two large companies to interview.

Two companies dominate the market for independent sulfur testing for the coal industry. We spoke with one of these testing companies in-depth and on numerous occasions. We also spoke with the second major coal testing company (briefly) to verify that their testing activities and procedures were similar.

Unlike the coal industry, which regularly hires independent laboratories to conduct sulfur tests for contracts, the majority of sulfur tests for petroleum products are conducted in-house. As such, independent petroleum-testing laboratories were not included in the interviews, and petroleum testing activities were investigated during our discussion with refineries.

Fossil Fuel Extraction and Processing

This industry consists of the coal processing industry, the petroleum refining industry, and the coke industry. We interviewed two coal companies. These companies represent 10 percent of total coal production. We found that the testing activities and procedures employed by this coal processing company were basically identical to those used by the coal testing laboratories.

We also interviewed three petroleum companies. Together, these companies account for 18 percent of U.S. revenues from petroleum products. Two of these companies are among the largest petroleum companies domestically and internationally. The third company we interviewed was a relatively smaller domestic producer. All of the respondents worked in research, development, and technology divisions.

We interviewed one integrated coke and steel company to obtain information on sulfur testing associated with coke production. The integrated coke and steel company interviewed produces and consumes in-house 11 percent of the total amount of coke produced domestically.

Fossil Fuel Combustion Industry

We interviewed three electricity-generating companies and one steel company. We selected companies that varied by size and that had purchased NIST SRMs.

From the same coke and steel company discussed earlier, we obtained information on the use of coke (and sulfur testing) in the production of steel. The steel company interviewed represents 12 percent of total national steel production. We also spoke with this industry's trade association, the American Iron & Steel Institute.

4.4.3 Data Collection Procedures

Our data were gathered from both primary and secondary sources. We used an interview guide to collect information from respondents via telephone interviews. Appendix B contains the interview guide. These guides were customized for each industry based on the hypotheses that we were testing for each industry. After we field-tested these questions, we collected data from respondents in four steps:

1. Make initial telephone contact.
2. Send respondent an overview of the project and the interview guide.
3. Conduct telephone interview.
4. Write-up interview and contact respondent again to ask clarifying questions if necessary.

We initially contacted a person at the target company who was referred by NIST or our consultants. If we determined that the initial contact was not qualified to address the issues of the survey, we contacted another individual recommended by the first contact. In some cases, we spoke with more than one person at a particular company. This was often necessary given the broad scope of the questions we asked.

We also gathered secondary information to support our analysis. This information was collected from government information agencies, trade associations, and industry literature.

5

Results

In Section 3, NIST's improvements in the methodology for measuring the sulfur content of fossil fuels and for certifying SRMs were discussed. These improvements increased the accuracy of available sulfur content information. In this section, we present data that documents the social benefits and cost associated with the use of NIST SRMs. Beginning in 1984, we quantified approximately $409 million in net benefits to society (NPV $1998) associated with the NIST sulfur SRMs.

The first step in quantifying the benefits from NIST sulfur SRMs, is to develop a counterfactual scenario from which the benefits and costs can be measured. As discussed in Section 3, our counterfactual scenario is that in the absence of NIST, the level of uncertainty associated with the measurement of sulfur in fossil fuels would today be similar to what it was prior to the introduction of IDMS in the middle 1980s. Based on this counterfactual assumption, we are able to express the impact of NIST SRMs in terms of a change in the standard error (SE) of sulfur measurement tests.

Table 5-1 shows the average ratio of SRM standard errors before and after the introduction of the IDMS methodology. Taking into account the percentage of measurement error associated with sampling, we determined that NIST SRMs improve measurement accuracy by a factor of about 1.75 for petroleum and 1.25 for coal. These factors represent the ratio of the counterfactual measurement errors to the NIST SRM measurement errors.

Table 5-1. Impact of NIST SRMs

Taking into account the percentage of measurement error associated with sampling, we estimate that NIST SRMs improve measurement accuracy by a factor of about 1.75 for petroleum and 1.25 for coal.

	Ratio of Counterfactual SE to NIST IDMS SE	Share of Measurement Error Associated with Sampling	Improved Measurement Accuracy Factor (Counterfactual/NIST)
Average for Petroleum SRMs	2.42	0.33	1.75
Average for Coal SRMs	1.60	0.85	1.25

The factors were derived by first determining the standard error, expressed as a percentage of the confidence interval, for all batches of SRMs. For each SRM, we developed the ratio of the standard error before and after NIST began solely using IDMS to certify SRMs. We then grouped the ratios by fuel type and developed two average ratios of the counterfactual SE to the NIST IDMS SE to represent petroleum and coal SRMs. These average ratios were then adjusted to account for the percentage of measurement error associated with sampling to obtain the improved measurement accuracy factor of 1.75 for petroleum and 1.25 for coal.

Table 5-2 presents summary annual data for the total and net benefits to society from NIST SRMs and NIST's expenditures. The time series begins in 1984 when the NIST Analytical Chemistry Division received a $40,000 internal standards development award to support research in new methods to certify SRMs. Benefits are first realized in 1986 because this was the first year the IDMS method was used in certifying sulfur SRMs and costs are projected through 2003 because industry representatives indicated that the IDMS method would remain the state-of-the-art technology in the near future.

Table 5-3 summarizes the NPV of the benefits associated with the six main hypotheses presented in Section 4. Of the six hypotheses, we are able to partially quantify the benefits for four hypotheses. Although we found anecdotal information to support the remaining hypotheses, little concrete evidence was available. Therefore, the potential benefits associated with these remaining hypotheses are discussed qualitatively, but they are not included in the estimates of economic return. In addition, industries' avoided expenditures on CRMs are included in the total benefit estimates.

Table 5-2. Annual Net Benefits to Society and NIST Expenditures
Approximately $409 million in net benefits to society (NPV $1998) were quantified associated with the NIST sulfur SRMs.

Year	Total Benefits	NIST Expenditures	Net Benefits to Society
1984	$—	$129,228	
1985	$—	$130,520	
1986	$17,274,061	$202,231	
1987	$17,964,227	$—	
1988	$18,675,304	$172,496	
1989	$19,120,623	$79,997	
1990	$20,291,709	$436,913	
1991	$20,250,116	$500,092	
1992	$20,226,198	$381,976	
1993	$19,510,225	$671,527	
1994	$66,801,079	$577,429	
1995	$68,502,832	$438,167	
1996	$73,033,742	$465,349	
1997	$76,610,716	$443,161	
1998	$79,960,879	$427,705	
1999e	$83,607,231	$449,575	
2000e	$87,402,088	$474,604	
2001e	$91,393,911	$501,013	
2002e	$95,593,819	$528,636	
2003e	$100,013,611	$558,362	
Total (NPV $1998)	$412,659,931	$3,657,834	$409,002,097

e = estimated

In the discussion that follows, both the qualitative and quantitative evidence that supports the analysis is discussed. We also present information about the costs of developing and applying the technology for developing SRMs. These costs include industry's costs for purchasing the SRMs and NIST's investment in the development and support of the analytical methods. Finally, several measures of economic return to NIST's investments are presented, including a benefit-cost ratio and social rate of return.

Table 5-3. Net Present Value of Benefits Hypothesis
Partial benefits in four of the six hypothesized categories were quantified along with avoided expenditures on CRMs. Not all the benefits in any individual hypothesis category were captured. For example, improved product quality benefits reflect only a subset of manufacturers in the supply chain. These benefits could not be extrapolated because of the diverse nature of the industries represented in the supply chain.

Hypothesis	NPV ($1998) of Benefit Hypothesis[a]
H1: Improved Product Quality	$2,665,422
H2: Change in R&D Costs	Not able to verify benefits
H3: Change in Transaction Costs	$7,542,201
H4: Improved Production Efficiency	$401,408,574
H5: Change in Regulatory Penalties	Transfer—not a net benefit to society
H6: Benefits to Environment	$78,449,207[b]
Avoided Expenditures on CRMs	$1,043,734
Total Benefits (NPV $1998)	$409,002,097

[a] Based on a 7 percent inflation adjusted social discount rate.

[b] Not included in total benefits summation in measures of economic return.

5.1 IMPROVEMENTS IN PRODUCT QUALITY (H1)

While SRMs clearly contribute to the quality of sulfur analysis instruments, CRMs, and sulfur testing methods, this improvement in quality is difficult to measure.

The first benefit hypothesis was that SRMs improve the quality of the products and services of the sulfur measurement industry, namely sulfur analysis equipment, CRMs, and sulfur analysis services. This hypothesis was investigated by asking respondents in the sulfur measurement industry

- whether the use of NIST SRMs affects the quality of their products,
- whether their customers specifically request the use of NIST SRMs in their quality control processes, and
- whether their customers are willing to pay a premium for products and services that are NIST-traceable.

The respondents answered this question in different ways.

5.1.1 Instrument Industry

Instrument manufacturers use NIST SRMs to conduct final tests and calibrations on their instruments. All respondents said that, if NIST standards were not available, they would use secondary standards, either prepared in-house or purchased externally, to provide these final checks. However, two of the four companies interviewed acknowledged that unavailability of a NIST standard to provide a universally accepted benchmark against which to test their instruments could affect the accuracy of their instruments, although they were not able to quantify this difference. Another respondent stated that he thought that in-house gravimetrically prepared standards were sufficient to meet the company's needs for quality control and calibration.

Of the four companies, two said that, if they did not use NIST SRMs, there could be an impact on customers' willingness to pay (WTP) for their products. Most CRM and instrument manufacturers mentioned their use of NIST SRMs in their marketing materials. Respondents noted that the use of NIST SRMs for quality control is expected and that NIST SRMs are generally treated as tacit industry standards for quality control programs. However, none of the companies we interviewed were able to quantify the impact of not using NIST SRMs on their customers' purchase decisions. They thought that the impact on customers' WTP would be minimal, particularly if no SRMs were available and all manufacturers used a substitute material. Thus, we were not able to quantify any benefits to the instrument industry from improved product quality or subsequent WTP.

5.1.2 CRM Industry

In the market for CRMs, NIST traceability is an important issue. Virtually all companies that manufacture or market sulfur standards for fossil fuels claim NIST traceability. This is an important selling point and a company trying to sell standards that are not certified as NIST-traceable would likely lose sales if competitors were selling NIST-traceable materials at a comparable price. We asked CRM companies if their customers' WTP for their products would change if they did not have an independent national standard against which to verify the quality of their products. Of the four companies we interviewed, three companies were not able to quantify potential sales if their products were not NIST-traceable. However, one company estimated that their customers' WTP would fall by about 25 percent if NIST standards were not available to verify the accuracy of their standards.

Using the formula presented in Section 4, we estimate the loss in consumer surplus from this company's products alone at about

$54,000 per year. Because the other companies we interviewed could not quantify the potential losses in WTP, we have not extrapolated these results to the remainder of the industry. This particular company positions itself in the high-quality end of the CRM market. Thus, although its customers may be willing to pay extra for the improved quality that NIST traceability provides, this may not be true for the customers of the other CRM companies.

5.1.3 Laboratories

Laboratories that conduct sulfur testing of coal, coke, and petroleum products routinely use NIST SRMs as part of their quality control program to verify the calibration of their instruments. While commercially prepared CRMs may be adequate for these purposes, some customers specifically request that NIST SRMs be used for these checks. Otherwise, laboratories typically use NIST SRMs once or twice per quarter. The customers that request NIST SRMs to be used for all calibration checks may be willing to pay a premium for their use in the quality control program.

One coal laboratory representative estimated the WTP premium associated with SRMs was about 5 percent. This company accounts for approximately 33 percent of sulfur coal testing industry revenues, which are approximately $2,220,000. Applying the 5 percent premium to industry coal testing revenue, we estimate that in 1998 the change in consumer surplus was about $313,000 for the entire coal testing industry. Table 5-4 presents the stream of benefits estimated for each hypothesis from when the IDMS method for sulfur was first introduced in 1986 and projected until 2003. To project benefits into the future, we used the average annual rate of sales growth. All data are presented in 1998 dollars.

Although we believe the change in consumer surplus for the petroleum testing industry to be proportional to that of the coal testing laboratories, we were unable to quantify that change. Because of the large number of firms that provide independent petroleum testing services and the wide range of other services they provide, we could not get an accurate estimate of the percentage of industry revenue generated by testing for sulfur in petroleum. Without these data, we could not determine a reliable estimate of the change in consumer surplus associated with using NIST SRMs in quality control programs.

Table 5-4. Estimated Annual Impacts of NIST Sulfur SRMs ($1998)

Avoided desulfurization of petroleum products and coal accounted for approximately 97 percent of total benefits.

Year	H1	H2	H3	H4 Coal	H4 Gasoline	H4 Diesel	H5	Avoided Expenditures on CRMs	Total Benefits
1986	$124,481	$—	$456,456	$16,693,125	$—	$—	$—	$—	$17,274,061
1987	$128,784	$—	$607,943	$17,227,500	$—	$—	$—	$—	$17,964,227
1988	$172,429	$—	$641,828	$17,818,125	$—	$—	$—	$42,922	$18,675,304
1989	$151,528	$—	$560,105	$18,388,125	$—	$—	$—	$20,865	$19,120,623
1990	$206,239	$—	$669,734	$19,295,625	$—	$—	$—	$120,112	$20,291,709
1991	$324,265	$—	$1,107,586	$18,675,000	$—	$—	$—	$143,266	$20,250,116
1992	$376,516	$—	$1,033,835	$18,703,125	$—	$—	$—	$112,722	$20,226,198
1993	$395,880	$—	$1,183,994	$17,726,250	$—	$—	$—	$204,101	$19,510,225
1994	$411,862	$—	$1,211,899	$19,378,125	$—	$45,619,197	$—	$179,996	$66,801,079
1995	$349,776	$—	$895,636	$19,368,750	$—	$47,748,215	$—	$140,456	$68,502,832
1996	$313,815	$—	$758,102	$19,948,125	$1,531,442	$50,328,686	$—	$153,574	$73,033,742
1997	$289,840	$—	$770,725	$20,435,625	$1,544,854	$53,419,039	$—	$150,632	$76,610,716
1998	$313,200	$—	$658,439	$20,975,625	$1,577,032	$56,286,887	$—	$149,697	$79,960,879
1999e	$348,086	$—	$730,176	$21,392,042	$1,600,361	$59,374,047	$—	$162,517	$83,607,231
2000e	$386,859	$—	$809,730	$21,816,727	$1,624,036	$62,588,301	$—	$176,435	$87,402,088
2001e	$429,950	$—	$897,951	$22,249,842	$1,648,061	$65,976,561	$—	$191,545	$91,393,911
2002e	$477,841	$—	$995,784	$22,691,556	$1,672,442	$69,548,247	$—	$207,949	$95,593,819
2003e	$531,067	$—	$1,104,276	$23,142,039	$1,697,183	$73,313,288	$—	$225,758	$100,013,611
Total NPV	$2,665,422	$—	$7,542,201	$180,186,303	$4,548,634	$216,673,636	$—	$1,043,734	$412,659,931

e= estimated

5.2 REDUCTIONS IN THE COST OF R&D (H2)

Our second hypothesis about the impact of NIST SRMs was that SRMs would reduce the cost of R&D to the sulfur measurement industry and the fuel industry by supporting accurate, reliable sulfur measurement. Although some of our interviewees indicated that NIST SRMs were part of their R&D laboratories' quality control program, they were not able to quantify any benefits to their R&D program from NIST SRMs. We have no evidence to support this hypothesis and cannot quantify any economic benefits due to reductions in the cost of R&D attributable to NIST SRMs.

5.2.1 Sulfur Measurement Industry

The companies that develop and manufacture instruments that measure sulfur content in fossil fuels use NIST SRMs in applications development and to verify their prototype instruments. Although all three of the instrument manufacturers we interviewed said that SRMs are used in the quality control process in these R&D laboratories, only one company stated that SRMs have any impact on the cost of conducting R&D. Furthermore, this company indicated that the R&D impact was minimal. The only savings the company representative could identify was the savings in terms of the labor required to gravimetrically prepare and verify in-house standards if NIST standards were not available. He could not quantify the associated cost savings.

5.2.2 Fossil Fuel Industry

The impact of NIST SRMs in the R&D sector of the fuel industry is minimal. Most petroleum companies conduct R&D in the development of lower sulfur fuels, but there is no evidence that NIST SRMs reduce the cost of this research. One representative mentioned that the primary reason that NIST SRMs are not an important factor in R&D is because a quick turnaround time for sulfur results is not as imperative in R&D as it is in production operations and purchase/sales situations. Because NIST SRMs support instrumental analytical methods that are used in quick-turnaround situations, they are much more important in these situations than they are in an R&D context.

5.3 REDUCTIONS DUE TO TRANSACTIONS COSTS (H3)

We hypothesized that NIST SRMs would reduce the cost of fossil fuel transactions because measurements are accepted as reliable; consequently, fewer transactions are disputed because of measurement error. Most of our contacts indicated that, theoretically, better measurements would reduce the number of disputes. However, they emphasized that, in actuality, disputes seldom occur and only a small proportion of them are related to sulfur measurement problems. To estimate the benefits attributable to NIST SRMs, we have to ask the question: what would be the increase in the number of disputes if sulfur measurements were less accurate in the absence of NIST?

To quantify this benefit, we first estimated the total cost to industry of measurement disputes and assumed that 5 percent of these disputes were associated with measurement error. We then used the change in the standard deviation of sulfur content measurement associated with and without the IDMS method to estimate the decrease in disputes attributable to NIST SRMs.

In the coal industry, the sulfur content of coal is specified in contracts. The acceptance levels are typically specified in pounds sulfur per million Btu or as the sulfur percent weight of coal. The contract generally details two sulfur specifications: a guaranteed monthly weighted average for sulfur content and a rejection limit sulfur content for individual shipments. For example, one industry representative indicated that a typical contact may specify that the average monthly sulfur content of their coal shipments cannot exceed 2.87 percent, and that if any individual shipment tested over 3.175 percent sulfur content, the shipment would be disputed and could be rejected pending the resolution of the dispute.

Disputes rarely occur. One coal laboratory respondent stated that less than 1 percent of all transactions are disputed. According to this estimate because there are roughly six million coal shipments each year in the United States, fewer than 60,000 shipments per year are disputed. A coal company respondent indicated that only "a few" shipments per year from her company are disputed. One electric utility told us that they handled five disputes per month, or about 120 disputes over coal shipments per year. Using the firm's share of annual electricity generation from coal, we can conservatively estimate the number of disputes per year to be about 2,200.

To estimate the benefits attributable to NIST SRMs, we have to ask the question, how much would this number rise if sulfur measurements were less accurate in the absence of NIST SRMs? As demonstrated in Section 4, if rejection criteria are constant, an increase in the size of the standard deviation associated with sulfur content measurement would increase the probability that a shipment may be disputed simply due to measurement error. For coal, the standard deviation today is only about 62 percent of what it was before the introduction of IDMS. Thus, we assume that the standard deviation of a sulfur measurement estimate would be 1.25 times as large without NIST SRMs as it would be with NIST SRMs.

Our model predicts that increasing the standard deviation by a factor of 1.25 increases the dispute probability from 0.035 percent to about 0.344 percent, meaning that about 18,800 more disputes occur due to measurement error. One electric utility respondent said the cost of resolving a dispute, inclusive of person-hours and laboratory expenses, is about $700. Using these estimates, for the coal supply chain, we estimate the cost of the additional disputes in the absence of NIST SRMs to be $13.2 million per year.

However, most of our respondents party to coal contracts said that usually when there is a dispute, it is because of human error. Thus, only a handful of the disputes that occur can be attributed to measurement error. No respondents were able to estimate the percentage of disputes attributable to measurement error. Assuming that 5 percent of the disputes are a result of measurement error, we estimate that the reduction in transactions costs because of increased measurement error is about $660,000 in 1998. Table 5-3 presents our estimates from 1986 until 2003. The data were weighted by the annual average percentage growth in sulfur SRM sales to coal companies, petroleum companies, electric utilities, and steel companies.

5.4 INCREASES IN PRODUCTION EFFICIENCY (H4)

Our fourth hypothesis is that NIST SRMs increase the efficiency of fuel blending, desulfurization, and equipment operations because the reliability of the measurement allows users to reduce the buffer they employ to ensure compliance with technical specifications. Information obtained during the interviews indicates that both the petroleum industry and the coal industry are beneficiaries of this benefit. In contrast, the interviews indicated that coke producers and electric utilities burning coal rarely adjust their buffers to take advantage of incremental gains in measurement accuracy because of the difficulty and cost of physically mixing coal.

5.4.1 Petroleum Industry

Petroleum refineries use buffers in their production processes to reduce the possibility of producing fuels that are found by regulatory agencies to be off-specification, which carries regulatory penalties for diesel nationally and gasoline in California. With NIST SRMs, refineries have more accurate information about the sulfur content of their products. The improved measurement accuracy allows refineries to reduce the buffer between their target sulfur content and the legal limit.

One petroleum industry respondent said that a typical refinery operates with a buffer of about 5 percent. For on-highway diesel fuel, which has a per-gallon sulfur content limit of 500 ppm, the targeted sulfur content is 475 ppm. This 475 ppm target sulfur content assures the refinery that, if the diesel fuel it produced is tested by a regulatory agency, it will most likely not have a sulfur content exceeding the 500 ppm critical limit.

The accuracy of NIST SRMs allow refineries to reduce their buffer, thereby saving on desulfurization costs. In the absence of NIST SRMs, the confidence interval around the target value widens because the standard error is larger—about 1.75 times what it is with NIST SRMs. Based on the approach outlined in Section 4, we estimate that to achieve the same level of confidence without NIST SRMs as with them, the target sulfur content would be 456.3 ppm, rather than 475 ppm. Thus, refineries would remove an additional 18.7 ppm from each gallon of on-highway diesel fuel if they did not have NIST SRMs. EPA estimates that the average cost of removing

1 ppm of sulfur from diesel and gasoline costs $0.0001 per gallon. Our petroleum industry contacts agreed with this estimate.

In 1998, over 30 billion gallons of on-highway diesel fuel were consumed in the United States. The cost of removing an additional 18.7 ppm sulfur from each gallon would have been approximately $56 million. Table 5-4 presents estimates beginning in 1994 because it was the first complete year in which on-highway diesel had a legal limit of 500 ppm. Estimates for 1999 until 2003 were generated using the average annual percentage growth in diesel sales from 1994 to 1998.

For gasoline, we limited our investigation to California reformulated gasoline. Currently, California is the only state where the sulfur content of gasoline is regulated. The regulation has been in effect since 1996.

Elsewhere, refineries may limit the amount of sulfur in gasoline to avoid damaging sensitive equipment, but they do not alter their production processes to conform to a legal limit, thereby avoiding regulatory penalties. Because these refineries alter their sulfur content levels at their discretion, it is difficult to determine their buffer and target sulfur content, and non-California reformulated gasoline was not included in the benefits calculations.

California Air Resources Board (CARB) limits the sulfur content of gasoline in California to an average of 30 ppm. Incorporating the 5 percent buffer, refineries producing gasoline for that market are targeting a 28.50 ppm sulfur content. In the absence of NIST SRMs, the refinery would have to revise its target limit downward to achieve the same level of confidence that they would not be caught off-specification. Refineries would target 27.38 ppm, removing an additional 1.12 ppm. In 1998, California consumed over 14 billion gallons of reformulated gasoline. If refineries had removed the additional sulfur, the additional cost would have been $1.6 million (see Table 5-4).

5.4.2 Coal Industry

The coal industry also uses buffers in their production process to ensure that delivered coal meets the sulfur content specified in contracts. Cleaning and blending of coal are used to remove sulfur prior to shipment.

One respondent from the coal industry estimates that coal processors typically use a buffer of 0.05 percent sulfur content. This buffer allows room for "spikes" in sulfur content but keeps the running average below the contract maximum. The coal cleaning process costs approximately $0.03 per ton per to remove 0.01 percent of sulfur.[1]

The accuracy of NIST SRMs allows refineries to reduce their buffer, thereby saving on coal cleaning costs. In the absence of NIST SRMs, the confidence interval around the target value widens because the standard error is larger—about 1.25 times what it is with NIST SRMs. Based on the approach outlined in Section 4, we estimate that, to achieve the same level of confidence without NIST SRMs as with them, the buffer would increase to 0.0625 percent sulfur content. Thus, coal processors would need to remove an additional 0.0125 percent sulfur from each ton of coal that they clean. This yields a cost savings of $0.0375 per ton associated with the increased accuracy of NIST SRMs.

It is estimated that the coal industry cleans approximately 50 percent of the 1.118 billion tons (1998) of coal mined in the U.S.[2] This yields an annual benefit of approximately $21 million in 1998 (see Table 5-4).

5.5 REDUCTIONS IN REGULATORY PENALTIES (H5)

Our fifth hypothesis was that NIST SRMs reduce the fines paid by industry due to environmental noncompliance because industry and the regulatory community have accurate and reliable sulfur content information. We hypothesized that improvements in the measurement of sulfur may reduce the incidence and quantity of penalties imposed by regulatory agencies.

As with coal transactions, the number of disputes between regulatory agencies and regulated entities, such as electric utilities and refineries, would probably rise in the absence of NIST SRMs.

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[1] Note that many factors influence the actual cost of removing sulfur from coal, such as whether the sulfur is in the coal or in the rock, aerability of the sulfur content, type of mine (underground or surface), type of cleaning process, and raw and clean coal storage capacity.

[2] A large share of western coal has a low enough sulfur content that it does not require cleaning.

Although this may be the case, the fines paid by industry to regulatory agencies constitute transfers payments. Therefore, we did not quantify the increase in the number of fines in the absence of NIST SRMs because no net social benefits are associated with transfer payments.

5.6 BENEFITS TO THE ENVIRONMENT (H6)

Our final hypothesis was that SRMs reduce the amount of sulfur entering the environment by providing industry greater control over the sulfur content of its fuels and by allowing compliance officials greater authority in enforcing the regulatory limits. Quantified benefits to the environment are not included in the total benefits presented in Table 5-4 or in the measures of economic return calculated in Section 5.9. These benefits are presented separately because they do not directly affect the sulfur measurement supply chain. However, they are estimated and shown in Table 5-5.

As with the production efficiency hypothesis, the benefits to the environment associated with NIST SRMs are limited to petroleum products. With NIST SRMs, the reproducibility interval around the target sulfur content value is smaller, which means that batches of diesel fuel and gasoline are released with less sulfur. Lower sulfur fuels reduce the amount of sulfur dioxide (SO_2) emitted to the environment.

Nationally, refineries produce diesel fuel with an average sulfur content target of 475 ppm. The reproducibility interval, in terms of ppm, is 64.32; the upper limit is the target plus half the reproducibility interval, or 507.16 ppm. If the refinery tests the sulfur content of the fuel and it is below this upper limit, they will release the fuel because they are confident that their fuel falls within the regulatory agency’s reproducibility interval around the 500 ppm legal limit. If the sulfur content exceeds the upper limit, the refinery will reblend the fuel rather than risk the regulators finding their product off-specification. In the absence of NIST, the reproducibility interval increases to 112.35 ppm because the standard error increases. The upper limit would be 531.17 ppm as opposed to 507.16 ppm. Thus, with NIST SRMs, gasoline is released with 24.01 ppm, or 5.06 percent, less sulfur.

Table 5-5. Benefits to the Environment ($1998)

Increased accuracy of sulfur measurement allows compliance officials greater authority in enforcing the regulatory limits. These benefits are not included in the measures of economic return calculated in Section 5.9 because they do not accrue directly to the sulfur measurement supply chain.

Year	H6 Gasoline	H6 Diesel
1984	$—	$—
1985	$—	$—
1986	$—	$—
1987	$—	$—
1988	$—	$—
1989	$—	$—
1990	$—	$—
1991	$—	$—
1992	$—	$—
1993	$—	$—
1994	$—	$18,181,234
1995	$—	$18,411,376
1996	$982,611	$19,101,802
1997	$997,147	$19,331,945
1998	$1,011,898	$19,792,229
1999^e	$1,026,868	$20,206,485
2000^e	$1,042,058	$20,620,741
2001^e	$1,057,474	$21,034,997
2002^e	$1,073,118	$21,449,253
2003^e	$1,088,993	$21,863,509
Total (NPV $1998)	$2,921,050	$75,528,157

e = estimated

According to EPA, SO_2 emissions from on-highway diesel fuel were 84,000 tons in 1997. Assuming a proportionate relationship between sulfur in diesel and SO_2 emissions, without NIST SRMs, 5.06 percent, or about 4,250 tons, more SO_2 would have been emitted to the environment. EPA estimates that, in the western

United States, the average environmental impact of a ton of SO_2 to be approximately $4,400 (1997).[3]

We estimate the benefits to the environment from NIST SRMs to be $19.8 million for diesel fuel in 1998. The same analysis for California gasoline yields approximately $1 million in benefits in 1998 (see Table 5-5). Benefits for both fuels begin in the first year in which there is a legislated sulfur content limit. Our benefits projections for 1999 to 2003 were based on the estimated growth in sulfur dioxide emissions associated with those fuels (EPA, 1997b).

5.7 INDUSTRY COSTS

Avoided expenditures on CRMs are modeled as a benefit and included in the total benefit calculation

When measuring the benefits of NIST SRMs, it is important to also take into account industry's avoided expenditures on CRMs.[4] It is assumed that in the absence of NIST SRMs industry would have been purchased commercially available CRMs to support their sulfur measurement needs. Thus, from society's perspective, these avoided CRM expenditures are treated as a benefit and included in the total benefit time series shown in Table 5-4.

CRMs are approximately 35 percent of the cost of NIST SRMs.[5] Based on this percentage, we assumed that expenditures by industry to produce CRMs would have been approximately 35 percent of NIST's production, operations, overhead, and administration expenditures.[6] Thus, in 1998 it is estimated that increased expenditures for CRMs in 1998 would have been approximately $150,000 in the absence of SRMs.

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[3] We believe this particular estimate to be more conservative because most estimates range from $2,000 to $13,000.

[4] Industry representatives said that no additional operational costs (pull costs) were associated with using SRMs compared to using CRMs.

[5] Excluding the prices for isooctane and lubricating oil standards, the average price of a NIST sulfur SRM is about $170. The pricing schedule for CRMs is based on the number of units purchased. Assuming that customers purchase CRMs in similar quantities as they purchase NIST SRMS, the average price is about $60. The $60 price was determined by averaging the prices for CRMs comparable to NIST SRMs from VHG Labs, Alpha Resources, AccuStandards, and NSI Solutions Thus, society's increased expenditures on sulfur CRMs is estimated to be approximately 170/60 = 35 percent of NIST's expenditures on sulfur SRMs.

[6] Research and development costs incurred by CRM manufacturers were assumed to be sunk costs and are not included in the industry's avoided CRM expenditures.

5.8 NIST EXPENDITURES

Beginning in 1984, NIST began incurring expenditures to support the Analytical Chemistry Division's development and use of IDMS sulfur SRMs. NIST expenditures are ongoing and cover SRM development, production, operations, overhead, and administrative costs for SRMs.

NIST's program expenditures over time for sulfur SRMs developed using the IDMS method are shown in Table 5-6. Expenditures were calculated from NIST's Standard Reference Market Transfer (SRMT) notices. The time series was developed using the following guidelines:

- ➤ SRM development costs are incurred in the first year of the time series.
- ➤ SRM production costs are incurred in the year in which the SRM "batch" was produced.
- ➤ SRM operating, overhead, and administration costs are distributed over time and are assumed to be incurred when individual SRMs are sold.

SRM development costs: NIST's Analytical Chemistry Division received a $40,000 internal standards development (SD) award in 1984 to support research in new methods to certify SRMs. Although this SD research was targeted toward certifying future metals SRMs, the methodology was directly transferable to fossil fuel analysis. Thus, 50 percent of this funding is ascribed to the fossil fuel standards certification program. This investment (adjusted for inflation) is shown in the NIST investment cost time series shown in Table 5-6.[7]

SRM production costs: Production costs were obtained from the SRMT notices and were available for 85 percent of the sulfur SRM "batches" (including new and reissued SRMs) produced between 1984 and 1998. Average unit production costs were $56 ($1998). Average unit production costs were used to estimate expenditures

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[7] Past NIST research conducted in related areas was also important to the development of sulfur SRMs. Sulfur SRMs have benefited from previous research in areas such as thermal ionization mass spectrometry (TIMS) developed for nuclear standards program and atomic weight research, sample preparation methods for TIMS, and sample preparation methods for isotope dilution. Costs associated with related/supporting research are not included in the NIST expenditure estimates presented in Table 5-6 used to calculate economic returns.

Table 5-6. Time Series of NIST Expenditures for Sulfur SRMs ($1998)
Production costs are incurred in the year in which the SRM was produced. SRM operations, overhead, and administrative costs are distributed over time and were assumed to be incurred when SRMs are sold.

Year	SRM Development Costs	SRM Production Costs	SRM Operations, Overhead, and Administrative Costs	Total Annual NIST Expenditures
1984	$31,918[a]	$97,310	$—	$129,228
1985		$130,520	$—	$130,520
1986		$202,231	$—	$202,231
1987		$—	$—	$—
1988		$157,496	$15,000	$172,496
1989		$59,642	$20,354	$79,997
1990		$319,402	$117,511	$436,913
1991		$226,284	$273,809	$500,092
1992		$75,627	$306,349	$381,976
1993		$283,951	$387,576	$671,527
1994		$158,254	$419,176	$577,429
1995		$101,383	$336,784	$438,167
1996		$162,653	$302,697	$465,349
1997		$121,530	$321,631	$443,161
1998		$161,553	$266,152	$427,705
1999		$169,043	$280,532	$449,575
2000		$178,914	$295,690	$474,604
2001		$189,357	$311,656	$501,013
2002		$200,311	$328,325	$528,636
2003		$212,119	$346,243	$558,362
Total NIST Expenditures (NPV $1998)	$31,918	$1,724,475	$1,901,442	$3,657,834

[a] $20,000 SD award in1984 converted to 1998 dollars.

for the remaining 15 percent SRMs, where SRMT notices information was not available and for projected SRMs. Projected SRM production from 1999 through 2003 was extrapolated based on the average number of SRMs produced in the 1990s.

SRM operating, overhead, and administration costs: These costs were also based on information obtained from SRMT notices, and average unit cost estimates were used when SRM information was not available. SRM operating costs are approximately \$90 per unit and account for approximately 95 percent of the operating, overhead, and administration category shown in column 4 of Table 5-6.

The total NPV (\$1998) of NIST expenditures, including SRM development, production, operations, overhead, and administrative costs, is \$3.4 million.[8] Production costs account for approximately 47 percent of NIST total expenditures.

5.9 CALCULATING MEASURES OF ECONOMIC RETURN

To determine the returns from NIST's investment in the development and operation of the sulfur SRM program, we compared the net benefits to industry described above with NIST sulfur SRM expenditures. We calculated three summary measures of the net benefits of the program: the benefit-cost ratio, the net present value (NPV), and the social rate of return.

If B_t is the total net benefits to industry (H1 through H5 plus avoided CRM expenditures) accrued to all beneficiaries in year t, and C_t is the cost to NIST of the program in year t, then the benefit-cost ratio for the program is given by

$$(B/C) = \frac{\sum_{i=0}^{n} \frac{B_{(t+i)}}{(1+r)^i}}{\sum_{i=0}^{n} \frac{C_{(t+i)}}{(1+r)^i}} \tag{5.1}$$

where t is the first year in which benefits or costs occur, n is the number of years the benefits or costs occur, and r is the social rate of discount. Because benefits and program costs may occur at different time periods, both are expressed in present-value terms before the ratio is calculated.

The NPV of the NIST SRMs program can be computed as

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[8] NIST recovers the majority of its SRM development, production, operations, overhead, and administrative expenditures by selling SRMs to industry. However, because we are estimating the benefits and costs of SRMs to society (not to individual organizations or economic sectors), the selling price of SRMs does not enter our analysis; the revenue recovered by NIST is a transfer payment.

$$NPV = \sum_{i=0}^{n} \left[\frac{B_{(t+i)}}{(1+r)^i} - \frac{C_{t+i}}{(1+r)^i} \right]. \tag{5.2}$$

The social rate of return is the value of r that sets NPV equal to 0 in Eq. (5.2).

For the NIST sulfur SRM program, the following parameter values were used to calculate economic returns:

t = 1984: first year in which NIST incurred development costs related to sulfur SRMs
n = 19: number of years from 1984 to 2003
r = 7 percent: inflation adjusted social discount rate

As shown in Table 5-2, NIST expenditures begin in 1984. However benefits associated with NIST sulfur SRMs are identified beginning in 1986 with the introduction of the IDMS sulfur SRM.

The three measures of economic return are provided in Table 5-7. The estimated net benefits to industry from the program greatly exceed NIST's investment costs. In addition, these estimates of economic return may represent a lower bounds because we were not able to quantify several identified benefit categories, whereas all identifiable costs to industry and NIST investment costs are included in the calculations.

Table 5-7. Economic Impact of NIST SRMs
Economic impacts reflect benefits and costs from 1984 projected through 2003.

Measure of Social Return[a]	Economic Impact
Benefit-to-cost ratio	113
Net present value ($1998)	$409,002,097
Social rate of return	1,056%

[a]Based on a 7 percent inflation adjusted social discount rate.

5.10 CONCLUSIONS

In summary, most industry representatives surveyed indicated that NIST SRMs have decreased the level of uncertainty associated with the measurement of sulfur in fossil fuels. In the absence of NIST SRMs, industry would likely purchase CRMs for sulfur testing. We found qualitative evidence that this reduction in the level of uncertainty has led to economic benefits throughout the supply chain, as described in the impact hypotheses presented in this section.

The majority of the economic benefits we were able to quantify are associated with using SRMs in petroleum refineries' and coal companies' production processes. Improved sulfur measurement allows these industries to reduce the amount of desulfurization they conduct on fuels, which yields substantial cost savings. Avoided desulfurization accounted for approximately 97 percent of the total benefits used to calculate measures of economic return.

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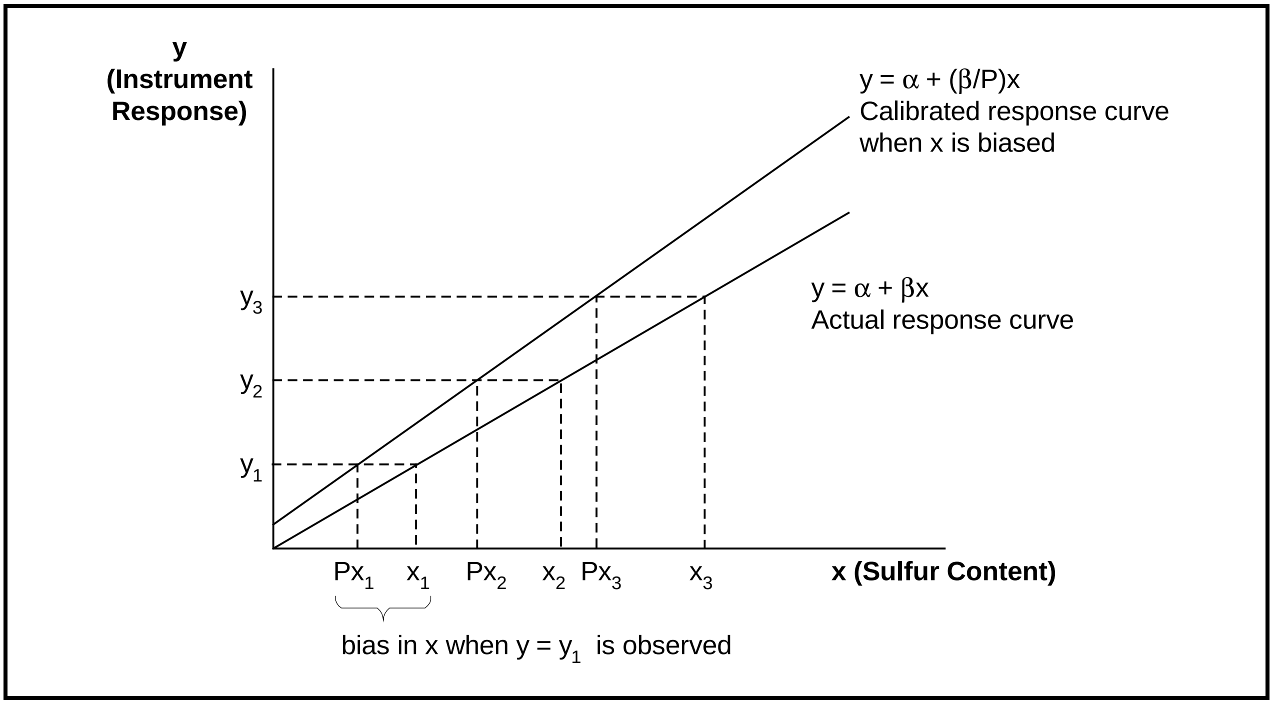
A

SRMs' Impact on Sulfur Measurement Accuracy

The instrumental methods used most often to measure the sulfur content of coal and petroleum products described above are based on the classic linear calibration model shown in Figure A-1. They rely heavily on the use of standards and calibrants. In this section, we demonstrate how the bias and precision of the standard used to calibrate the instrument contribute to uncertainty in sulfur content measurement.

Figure A-1. Classical Linear Calibration Model

Bias in the calibration standard leads to bias in the estimate of the slope of the curve; this leads to bias in estimates of the sulfur content.



The instrument response curve can be described as

$$y_i = \alpha + \beta x_i + \varepsilon_i,$$

where

y_i is the reported value of the sulfur content for test i, and

x_i is the actual (or accepted) value of the sulfur (as defined by the standard) for test i.

If we assume that x_i, the amount of sulfur in the standard, is known with certainty, then the error term, ε_i, refers only to measurement error associated with the instrument response. If we also assume that all the other assumptions of ordinary least squares (OLS) apply, the OLS estimator of β, $\hat{\beta}$, is an unbiased, consistent estimator of the slope of the calibration curve. The error ε_i indicates the uncertainty associated with the measurement of a single sulfur sample using that instrument.

This is the classic linear calibration model. We assume that this form of the model applies. It relies on the assumption that the calibration curve is linear, at least locally. In many cases, the calibration is conducted at several points along the line to allow the linearity to be tested. The issue of the appropriateness of this assumption is discussed at length by Mandel (1984).

A.1 IMPACT OF BIAS IN THE CERTIFIED VALUE OF THE SRM

Now suppose that the standard values of x are not known with certainty. First, assume that x_i', the certified sulfur content of the standard, is really equal to Px_i, where x_i is the actual value and P is a given proportion that holds for all standards. Note that

$$P = \frac{\%\text{ recovery}}{100} = \frac{x_i'}{x_i} = \text{relative bias} + 1 = \frac{\text{bias}}{\text{true } x_i} + 1.$$

The calibration curve gives

$$\begin{aligned} y &= \alpha + \beta x + \varepsilon \\ &= \alpha + \frac{\beta}{P} x' + \varepsilon. \end{aligned}$$

Thus a negative bias in the SRMs ($P<1$) leads to an overestimate of β, which in turn leads to negative bias in the observed concentrations that mimics the bias in the SRMs:

$$x' = \frac{y - \alpha}{\beta / P} = P\left(\frac{y - \alpha}{\beta}\right) = Px.$$

A.2 RANDOM MEASUREMENT ERROR IN THE CERTIFIED VALUE OF THE SRM

Now consider the impact of random measurement error associated with x_i. Putting aside the issue of bias in the calibration standard, let us assume that there is no bias in x_i (e.g., the certified value of the standard is equal to the expected value), but that the certified value is measured with error. In this case, two things happen:

1. The error associated with the measurement of x_i introduces additional error into estimates of y_i.
2. The least squares estimate of the slope underestimates the true value (Maddala, 1988). This is the classic errors in variables model. The bias is equal to $\beta\lambda$, where λ is the proportion of error variance in the variance of x_i. This bias occurs because the usual OLS assumption of independence is violated (the equation error ε_i is correlated with the x_i).

Assume that the variability of the observed instrument responses during the calibration process can be separated into two components:

$$\sigma_{e_y}^2 + \beta^2 \sigma_r^2 ,$$

where $\sigma_{e_y}^2$ is the variance associated with the instrument response, and σ_r^2 is the variance associated with the SRM. Then the variance of an observed sulfur value, X_1,

$$\mathrm{Var}(X) = \frac{\sigma_{e_y}^2}{\beta^2} + \sigma_r^2 = \sigma_{e_x}^2 + \sigma_r^2 ,$$

where $\sigma_{e_x}^2$ is the error variance translated into the x scale that would be expected with perfect SRMs. This formula treats the slope as a known quantity (i.e., it ignores random error in the estimate of the slope). In practice, the two variance components may be inseparable; that is, we may not be able to determine what part of the variance is due to variability in the SRM.

However, recall also that petroleum products and coal must be sampled before analysis and that sampling introduces another source of uncertainty. Suppose the material (coal or petroleum) is sampled from a batch. The result of the sulfur analysis is the mean of n observations of the sulfur content of the batch. Then the variance of the mean of n observations ($\bar{x}$) is:

$$\mathrm{Var}\,(\bar{X}) = \frac{(\sigma_s^2 + \sigma_{e_x}^2 + \sigma_r^2)}{n}\ .$$

Note that if the samples that are taken are composites (e.g., samples taken from a number of locations and mixed up to make a single sample—this is common in coal sampling), then the equation is

$$\mathrm{Var}\,(\bar{X}) = \frac{\left(\frac{\sigma_s^2}{k} + \sigma_{e_x}^2 + \sigma_r^2\right)}{n},$$

where k is the number of samples in the composite and n is the number of composite samples. This formula assumes that the compositing process itself has negligible error; this assumption will tend to be violated if the physical size of the composite gets too large (i.e., if k is “too big”) and/or if homogenization or weighing is difficult.

B Survey Form

This appendix contains a master list of the survey questions for primary data collection from industry. We constructed ten different interview guides—one for each of the industries listed in Table B-1. After we finalized the master list of questions, we developed each interview guide by pulling the relevant sections, as shown in Table B-1, from the master list into the guide.

Table B-1. Structure of Industry Interview Guides
We will construct each of the ten interview guides by pulling relevant sections from the master list of questions.

Industry	Relevant Questionnaire Sections
Sulfur measurement industry	
Instrument manufacturers	1, 2, 3, 4.1, 4.2
CRM manufacturers	1, 2, 3, 4.1, 4.2
Independent testing laboratories	1, 2, 3, 4.1, 4.2
Fossil fuel extraction, processing, and transportation industry	
Coal companies	1, 2.3, 4.3, 4.4
Petroleum companies	1, 2, 3, 4.1, 4.3, 4.4
Coke companies	1, 2, 3, 4.3, 4.4
Oil pipelines	1, 2, 3, 4.3, 4.4
Fossil fuel combustion industry	
Electricity generation firms	1, 2, 3, 4.3, 4,4
Steel companies	1, 2, 3, 4.2, 4.3, 4.4
Regulatory agencies	1, 2, 3, 4.3, 4.5

1.1 Contact Information

1.1.1 Contact name:

1.1.2 Contact address:

1.1.3 Contact phone:

1.1.4 Contact fax:

1.1.5 Contact email:

1.1.6 Date and time of interview:

1.2 Company Information

1.2.1 Company name:

1.2.2 Division and title of contact:

1.2.3 Contact background:

1.2.4 Company's primary line of business:

1.2.5 Company's total revenue:

1.2.6 Division revenue (if applicable)

1.2.7 List of company products and services that are supported in any way by SRMs or sulfur testing (might have to ask this later in the interview so the interviewee understands purpose and context of question)

Product Description	Price	Annual Revenue, or Percent of Total Revenue

2. USE OF SULFUR TESTING AND SRMS

2.1 Use of Sulfur Testing

2.1.1 Does your company conduct tests of the sulfur content of fossil fuels?

2.1.2 What fuels are tested?

2.1.3 How many tests do you conduct each day?

2.1.4 What is this information used for?

2.1.5 What ASTM methods are followed in this testing?

Check if Used	ASTM Method Number	Description
	D 4239 (Method C)	Sulfur in the Analysis Sample of Coal and Coke Using High-Temperature Tube Furnace Combustion Methods
	D 2622	Sulfur in Petroleum Products by X-Ray Spectrometry
	D 5453	Determination of Total Sulfur in Light Hydrocarbons, Motor Fuels, and Oils by Ultraviolet Fluorescence
	ASTM D0129	Sulfur in Petroleum Products (General Bomb Method)
	ASTM D1072	Sulfur Content (Total) In Fuel Gas
	ASTM D1266	Sulfur in Petroleum Products (Lamp Method)
	ASTM D1275	Corrosive Sulfur in Electrical Insulating Oils
	ASTM D1552	Sulfur in Petroleum Products (High Temperature Method)
	ASTM D2784	Sulfur in Liquefied Petroleum Gases by Oxy-Hydrogen Burner/Lamp Test
	ASTM D3120	Sulfur in Liquid Petroleum Products by Oxidative Microcoulometry
	ASTM D3177	Sulfur(Total)—Analysis Sample of Coal/Coke For Ultimate Analysis
	ASTM D3227	Mercaptan Sulfur in Gasoline, Kerosene (Potentiometric Method)
	ASTM D3246	Sulfur in Petroleum Gas By Oxidative Microcoulometry
	ASTM D4045	Sulfur in Petroleum Products by Hydrogenolysis and Rateometric Colorimetry

Check if Used	ASTM Method Number	Description
	ASTM D4294	Sulfur-Petroleum Products, by Energy-Dispersive X-ray Fluorescence Spectroscopy
	ASTM D4468	Sulfur Content (Total) in Gaseous Fuels, by Hydrogenolysis/Rateometric Colorimetry
	ASTM D4951	Additive Elements-Lubricating Oils by Inductively Coupled Plasma Atomic Emission Spectrometry
	ASTM D4952	Active Sulfur Species-Fuels/Solvents, Qualitative Analysis by Doctor Test
	ASTM D5016	Sulfur Trioxide (SO_3) in Ash From Coal/Coke Using High Temperature Tube Furnace Combustion Method with Infrared Absorption
	ASTM D5504	Sulfur Compounds—Presence in Natural Gas/Gaseous Fuels, by Gas Chromatography/Chemiluminescence
	ASTM D5623	Sulfur Compounds in Light Petroleum Liquefy Gas Chromatography

2.1.6 What instruments do you use in these tests?

Company	Model Number	Description

2.2 Use of SRMs

2.2.1 What calibrants do you use with these instruments/methods?

2.2.2 Do you use NIST SRMs? (Before interview, check against NIST SRM Customer Database.)

2.2.3 How many years have you been using NIST SRMs?

2.2.4 Which SRMs do you use? (Check against table below.)

Certificate Date	1st Year Used	SRM Number	Description
9/1/95		1616a	Sulfur in Kerosene
7/1/95		1617a	Sulfur in Kerosene
4/30/91		1619a	Sulfur in Residual Fuel Oil, 0.7%
7/27/98		1619b	Sulfur in Residual Fuel Oil, 0.7%
7/1/90		1620b	Sulfur in Residual Fuel Oil, 4%
7/1/96		1621e	Sulfur in Residual Fuel Oil, 1%
4/1/97		1622e	Sulfur in Residual Fuel Oil, 2%
7/1/96		1623c	Sulfur in Residual Fuel Oil, 0.3%
6/1/97		1624c	Sulfur in Distillate Fuel Oil, 0.4%
6/1/97		1632b	Trace Elements in Coal (Bituminous)
6/1/93		1633b	Trace Elements in Coal Fly Ash
7/1/95		1635	Trace Elements in Coal (Subbituminous)
4/1/94		1819a	Sulfur in Lubricating Base Oil
3/1/98		2294	Reformulated Fuels (nom. 11% MTBE, 35 mg/kg sulfur)
3/1/98		2295	Reformulated Fuels (nom. 15% MTBE, 300 mg/kg sulfur)
3/1/98		2296	Reformulated Fuels (nom. 13% ETBE, 35 mg/kg sulfur)
3/1/98		2297	Reformulated Fuels (nom. 10% ethanol, 300 mg/kg sulfur)
5/1/94		2682a	Sulfur in Coal, 0.5%
		2683a	Sulfur in Coal, 2%
10/27/97		2683b	Sulfur in Coal, 2%
12/1/97		2684a	Sulfur in Coal, 3%
5/1/94		2685a	Sulfur in Coal, 5%
12/1/93		2690	Trace Elements in Coal Fly Ash
12/1/93		2691	Trace Elements in Coal Fly Ash
9/1/94		2692a	Sulfur in Coal, 1%
10/1/90		2717	Sulfur in Residual Fuel Oil

Certificate Date	1st Year Used	SRM Number	Description
NA		2718	Green Petroleum Coke
NA		2719	Calcined Petroleum Coke
8/1/95		2724a	Sulfur in Distillate Fuel Oil, 0.04%
5/1/97		2775	Foundry Coke
3/1/98		2776	Furnace Coke

2.2.4 How do you use the NIST SRMs?

2.2.5 Do you use any secondary standards?

If Yes, which do you use? (Fill in table below.)

Company	CRM Number/Name

2.2.6 How do you use the secondary standards, and how does this differ from how you use NIST SRMs?

2.2.7 What do you view as the difference between NIST and secondary standards?

- Quality?
- Price?
- Best use?

3 IMPACT OF SRMS

3.1 Suppose NIST SRMs were not available for the uses described above. What would you use as a substitute?

3.2 Given that you would have to substitute a different material or process, do you think the methods you use to measure sulfur in fossil fuels would change?

- By what percentage do you think the repeatability of ASTM methods would change?
- Do you think the level of bias would change?

4 USE OF SULFUR TESTING INFORMATION

4.1 R&D

4.1.1 Does your company conduct R&D related to sulfur content of fuels or the development of sulfur measurement instruments and methods?

4.1.2 What is your company's total R&D budget?

4.1.3 What percentage of your company's total R&D budget is allocated to sulfur testing or sulfur content issues?

4.1.4 How do NIST SRMs support this R&D?

4.1.5 In the absence of NIST SRMs, do you think your R&D costs in this area would be higher?

- By what percentage?
- Why?

4.2 Quality of Products and Services

4.2.1 Do you use NIST SRMs for quality control or for any other reason in the production of your products and services?

4.2.2 If NIST SRMs were not available, what changes would you make in these processes?

4.2.3 How do you think this would affect the quality of your products?

4.2.4 Do you think your customers would value your products less if they were not produced with the support of or traceability to NIST SRMs?

4.2.5 Given the current prices of your goods and services, by what percentage do you think the prices your customers would be willing to pay for your goods and services would fall?

4.3 Transactions Costs

4.3.1 What percentage of the transactions (sales or purchases) of fossil fuels are based on contracts that specify sulfur content?

4.3.2 How are these contracts structured?

4.3.3 What happens if the contract specifications are not met?

- What happens if the sulfur content is too high?
- What if it is too low?

4.3.4 How often are shipments disputed due to sulfur content?

4.3.5 Are these disputes usually resolved?

4.3.6 How are they resolved?

4.3.7 How are SRMs used in the dispute settlement process?

4.3.8 What is your estimate of the cost of resolving a dispute?

- What are the most costly parts of the process?

4.3.9 How often are shipments totally rejected (i.e., no resolution of dispute)?

4.3.10 What could help to decrease the incidence of these disputes?

4.3.11 Do you think these disputes or rejections are ever caused by measurement error?

4.3.12 What percentage of disputes do you think could be avoided if the measurement process was more accurate?

4.4 Productivity

4.4.1 What operations at your facility are affected by sulfur content?

- Fuel blending
- Desulfurization
- Boiler operations
- Emissions control
- Coking
- Others?

4.4.2 How are they affected by sulfur content?

4.4.3 What are the technical specifications regarding sulfur content of fuels for these processes?

4.4.4 Do you feel that the information you have about sulfur content is sufficient to ensure that you meet the technical specifications for sulfur?

4.4.5 How often are the technical specifications not met?

4.4.6 What is the impact of going over technical limits?

- What are the technical impacts?
- What are the economic impacts?

4.4.7 What is the impact of going under technical limits?

- What are the technical impacts?
- What are the economic impacts?

4.4.8 What is your strategy for ensuring that you meet the technical limits?

4.4.9 Do you use a "buffer," i.e., shoot for some lower level to ensure that, given measurement error, you will not test over the limit?

4.5 Regulatory Penalties

4.5.1 How are sulfur content limits monitored?

4.5.2 What is the structure of enforcing these limits?

- Under what conditions are regulatory penalties imposed?
- What is the size of the regulatory penalties?
- How many companies are fined per year, and what is the annual amount of total fines?

4.5.3 What is the role of NIST SRMs in imposing regulatory penalties?

4.5.4 How would enforcement be affected if NIST SRMs were not available to support the measurement process?

C Profiles of Affected Industries

This appendix provides the background required to understand the importance of NIST SRMs to this supply chain. Section C.1 provides brief profiles of the affected industries: the sulfur measurement industry, the fossil fuel extraction and processing industry, and the fossil fuel combustion industry. Section C.2 describes the importance of sulfur as a characteristic of fossil fuels, including the regulations affecting the industries that produce and use fossil fuels in the U.S., and why these regulations increase the importance of accurate information about the sulfur content of fossil fuels. Section C.3 describes how NIST SRMs support these industries, including information about who buys NIST SRMs for sulfur in fossil fuels and how they are used.

C.1 INDUSTRY PROFILE

Many industries depend on NIST SRMs to support the measurement of sulfur in fossil fuels. Figure C-1 provides a graphical representation of the relationships among these industries. The sulfur measurement industry includes manufacturers of sulfur measurement instruments and CRMs and independent laboratories that conduct sulfur analysis. These companies use NIST SRMs in developing their instruments, preparing their CRMs, and providing quality control in their sulfur measurement laboratories. They supply instruments, reference materials, and analytical services to the fossil fuels industry.

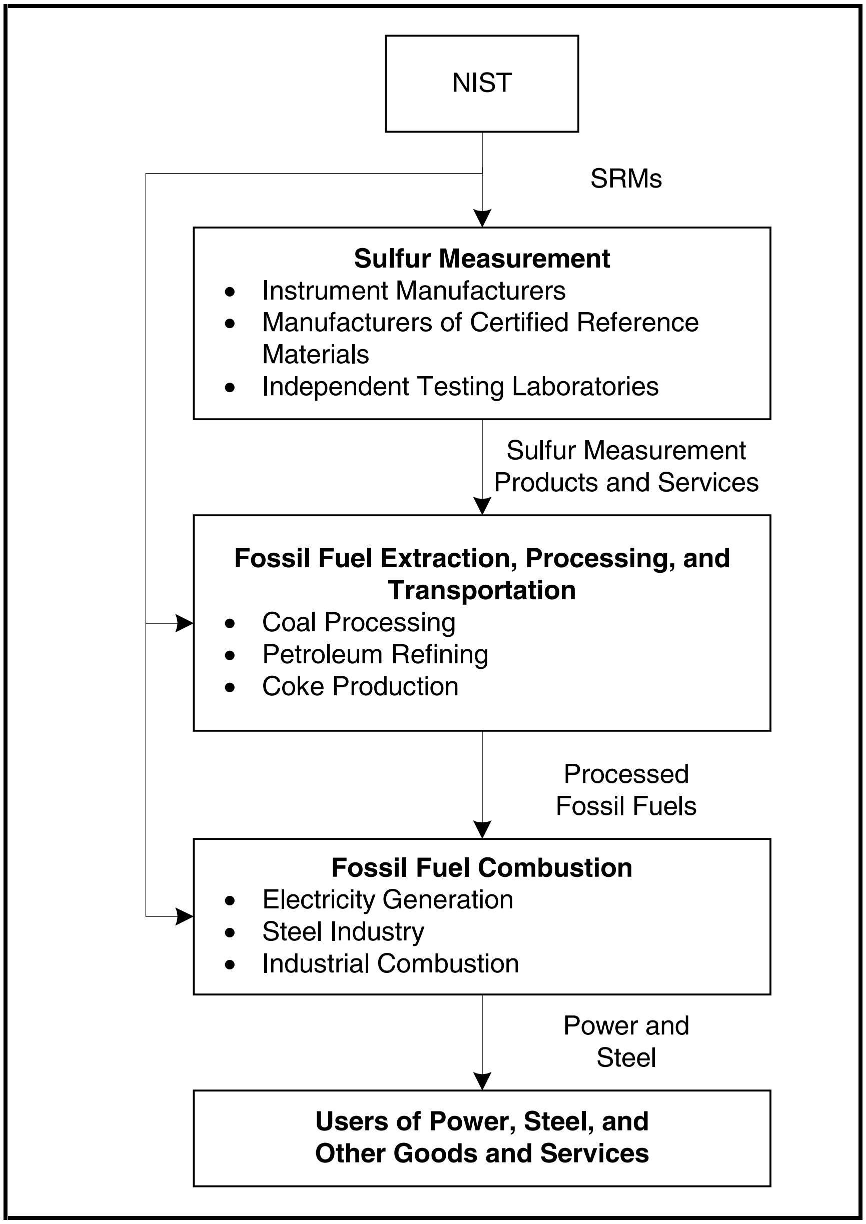


Figure C-1. Industries Affected by Measurement of Sulfur in Fossil Fuels
Sulfur measurement is supported by each element of the measurement industry and is used by each member of the fossil fuel supply chain.

The fossil fuels extraction and processing industry includes coal processing, petroleum refining, and coke production.[1] This industry uses the sulfur measurement products and services of the sulfur measurement industry and also uses NIST SRMs to support their in-house sulfur measurement activities. This industry supplies

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[1] Although natural gas is part of the fossil fuel industry, we did not analyze the natural gas industry because NIST does not provide an SRM for sulfur in natural gas because very little sulfur is found in natural gas, and its measurement is not an important industry issue.

processed fossil fuels to the industries that engage in fossil fuels combustion.

Although many industries engage in the combustion of fossil fuels, we concentrated on three sectors—sulfur measurment industry, petroleum refining, and coal processing—because they are primary users of fossil fuels. These industries use NIST SRMs for their in-house sulfur measurement activities. Industrial combustion also accounts for a large percentage of the fossil fuels consumed in the U.S. However, because of the difficulty of characterizing this diverse set of industries, we focus primarily on the electricity industry and the steel industry in this study.[2]

The final link in the supply chain is the users of power, steel, and other goods and services that are produced with fossil fuels. This link includes essentially the entire U.S. economy. Thus, we limited our analysis by focusing on the upstream components of the supply chain.

Environmental regulatory agencies, including EPA and state agencies, affect the operations of the second and third tier of industries. They develop, monitor, and enforce sulfur content regulations for the petroleum industry and develop, monitor, and enforce sulfur compound emissions limits for industries engaging in fossil fuel combustion. We discuss the role of the regulatory community and their use of NIST SRMs in Section C.2.

C.1.1 Sulfur Measurement Industry

The industry that supports the measurement of sulfur in fossil fuels includes the manufacturers of instruments, suppliers of CRMs, and independent laboratories that conduct sulfur analysis.

Instrument Manufacturers

Determinators, spectrometers, elemental analyzers, and chromatographers are measurement equipment used to determine the elemental composition of organic and inorganic samples. Fuel and chemical manufacturers for whom knowledge of a sample's sulfur content is important use these devices. For example, the

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[2] Industrial combustion refers to the use of industrial, commercial, and institutional (ICI) boilers whose primary use is for process heating, electrical or mechanical power generation, and/or space heating. Industrial boilers are used in all major industrial sectors.

petroleum industry uses sulfur analyzers to determine the sulfur content of the fuels they produce.

Manufacturers and consumers of these measurement instruments use NIST's sulfur SRMs to test and calibrate their equipment. These instruments must be properly calibrated to provide quality laboratory results. Sulfur SRMs allow technicians to test an instrument's accuracy and inform them of any need for adjustments. Equipment technicians may use NIST's sulfur SRMs directly, or they may use NIST-traceable CRMs from a secondary manufacturer to calibrate laboratory equipment.

Although many companies manufacture laboratory equipment, relatively few manufacture the type of equipment used to determine the sulfur content of coal and petroleum products. Table C-1 lists companies that produce these instruments at manufacturing facilities in the U.S. Together, these companies generate over $1 billion in revenue, although a significant percentage of this revenue is from equipment other than sulfur analysis equipment. Smaller firms generally produce a single product or several models of a single product, such as a line of analyzers. Many larger firms also manufacture other laboratory equipment, such as analyzers for nitrogen or other elements.

Manufacturers of Certified Reference Materials

A CRM is defined by the International Standards Organization (ISO) as "a reference material one or more of whose property values are certified by a technically valid procedure, accompanied by or traceable to a certificate or other documentation which is issued by a certifying body" (American National Standards Institute [ANSI], 1981). CRMs are used in the same way as NIST SRMs—for equipment calibration, development of other standards, and quality control for analyzing sulfur in fossil fuels. CRMs are often used in conjunction with NIST SRMs. In many laboratories, CRMs are used on a daily basis while NIST SRMs are used only occasionally.

Table C-2 lists the companies that market CRMs for sulfur in fossil fuels in the U.S. Each company's role in the production of their CRMs varies. Some companies produce and certify CRMs at their own facilities and laboratories, whereas other companies produce the standards but hire an outside laboratory to certify the sulfur

Table C-1. Principal Manufacturers of Sulfur Analysis Equipment
The market for sulfur analysis equipment includes a few very large firms and many smaller firms.

Company	City	State	Sales ($million)[a]	Employees	Year[b]
Alcor Petroleum Instruments, Inc.	San Antonio	TX	8.00	35	1997
Amray, Inc. (KLA-Tencor)	Bedford	MA	20.00	185	1996
Analytical Spectral Devices	Boulder	CO	4[c]	27	1997
Antek Instruments Co.	Houston	TX	8.00	50	1997
Asoma Instruments, Inc.	Austin	TX	15.00	70	1998
Berger Instruments, Inc.	Berwyn	PA	1.00	35	1997
Buck Scientific, Inc.	Norwalk	CT	8[c]	30	1998
Burrell Scientific, Inc.	Pittsburgh	PA	4.00	18	1997
Diano Corp.	Woburn	MA	2.00	14	1997
Exeter Analytical, Inc.	N. Chelmsford	MA	1.00	5	1997
Extrel Corporation	Pittsburgh	PA	14.00	108	1997
Hitachi Instruments	San Jose	CA	77.4[b]	280	1997
Horiba Instruments (USA), Inc.	Irvine	CA	81.00	250	1997
Houston Atlas	Houston	TX	7.50	40	1998
Kevex Instruments	Valencia	CA	22.00	130	1997
Koehler Instrument Co., Inc.	Bohemia	NY	4.00	NA	1997
Leco Corp.	St. Joseph	MI	100.00	1,000	1992
Leeman Labs, Inc.	Lowell	MA	17[c]	125	1998
Nicolet Instrument Corp.	Madison	WI	48.00	400	1997
Noran Instruments, Inc.	Middleton	WI	40.00	160	1997
Oxford Instruments America, Inc.	Concord	MA	12[d]	80	1997
Preiser Scientific, Inc.	St. Albans	WV	8.00	40	1997
Spectro Analytical, Inc.	Littleton	MA	9[d]	22	1997
Varian, Inc.	Palo Alto	CA	557.8[c]	3,033	1998

[a] Sales and employment data are from American Business Information, Inc., 1998. The American Business Disk [computer file]. Omaha, NE: American Business Information (except where indicated).

[b] Year for which sales and employment data are applicable.

[c] Sales and employment information for these companies is from Information Access Corporation, 1998. Business Index [computer file]. Foster City, CA: Information Access Corporation.

[d] Sales and employment information is from Dun & Bradstreet, 1997. *D&B Million Dollar Directory: America's Leading Public and Private Companies*. Bethlehem, PA: Dun & Bradstreet, Inc.

Source: This list of companies was compiled from various public sources on the instruments market.

Table C-2. Sulfur in Fossil Fuels CRM Manufacturers' Sales Ranges and Employment, 1999
This industry comprise small- to medium-size companies.

Company	City	State	Sales ($million)	Employment
Absolute Standards, Inc.	Hamden	CT	0.90[a]	7
AccuStandards, Inc.	New Haven	CT	4.65[a]	50
Alpha Resources, Inc.	Stevensville	MI	15.00	22
Analytical Services, Inc.	The Woodlands	TX	0.30[a]	2
NSI Chemical Standards, Inc.[b]	Durham	NC	3.75	17
SPEX CertiPrep, Inc.[b]	Metuchen	NJ	10.00[c]	NA
Vanguard Solutions, Inc.	Ashland	KY	0.78[a]	3
VHG Labs, Inc.	Manchester	NH	1.75	19

[a] Dun & Bradstreet, 1999. *D&B Million Dollar Directory: America's Leading Public and Private Companies.* Bethlehem, PA: Dun & Bradstreet, Inc.

[b] These companies market CRMs but outsource the preparation and certification of sulfur CRMs.

[c] Information Access Corporation. 1998. Business Index [computer file]. Foster City, CA: Information Access Corporation.

Source: American Business Information, Inc. 1998. The American Business Disk [computer file]. Omaha, NE: American Business Information.

content. A third option for companies is to purchase standards from another firm and then market those standards under their own private label.

CRMs are generally prepared using NIST SRM products (when available) and the American Society for Testing and Materials (ASTM) procedures. However, none of the CRM producers duplicate the procedures followed by NIST. NIST SRMs for sulfur in fossil fuels are certified using a technique known as IDMS. As explained in Section 3, IDMS is a definitive method that virtually eliminates bias and significantly reduces the relative uncertainty associated with reference materials. No commercial CRM manufacturers use IDMS; instead, they employ ASTM methods and/or interlaboratory testing for certification. The less rigorous process used by the CRM manufacturers can sometimes lead to significant differences between the accuracy and precision of the certified values provided by NIST and those provided by a CRM manufacturer.

Many CRM companies offer a wider variety of standards than NIST does. They may also provide a wider variety of base materials as well as a larger selection of concentrations. Those CRMs that do have a NIST SRM counterpart usually cost less than the comparable NIST SRM. The price difference probably reflects differences in the cost of instruments and procedures used to certify the reference materials and economies of scale associated with CRMs' larger production volume.

NIST SRMs are an important input in the CRM production process. CRM manufacturers use NIST SRMs to verify product quality and to certify that their products are NIST-traceable. It is possible that CRMs would be more expensive to produce and would not be of the same quality if NIST SRMs were not available. Many CRM manufacturers use the fact that their products are NIST-traceable as a key selling point.

Eight small- to medium-sized companies market CRMs for sulfur in fossil fuels (see Table C-2). The smallest companies have annual revenues as low as $300,000; the largest have annual revenues as high as $15 million. As a group, these companies had combined annual revenues of about $37 million in 1997. Only two companies employ more than 20 people: Alpha Resources and AccuStandards.

Independent Sulfur Testing Laboratories

Independent sulfur testing laboratories fall within SIC 8734, testing laboratories. In 1992, the U.S. had over 4,500 commercial testing laboratories generating almost $5 billion in revenue and $2 billion in payroll each year (U.S. DOC, 1994).[3] A small subset of these laboratories conduct sulfur analysis of fossil fuels. These laboratories conduct inspection, sampling, and analytical services for fossil fuel producers and consumers.

Independent laboratories are an important link in the supply chain because they provide independent testing results to satisfy contractual requirements for fossil fuel transactions.

Independent laboratories are an important link in the supply chain affected by SRMs. Although many mines, coking plants, coal preparation plants, utilities, and refineries have their own laboratories for these analyses, independent laboratories are becoming more important, particularly for contractual matters. Third-party independent laboratory results are routinely used to satisfy contractual requirements for buyers and sellers in the coal

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[3] These figures include taxable firms only. Noncommercial research organizations are not included.

industry, and this arrangement is increasing in the petroleum industry as well. To cut costs some firms also hire independent laboratories rather than operate their own.

Independent testing laboratories offer coal and petroleum sampling and testing services. They also offer an array of other services:

- the running of contract laboratories;
- coal preparation plant services: consulting on preparation plant development, operation, equipment, washability, and best practices;
- power plant services: consulting on fuel combustion, performance testing, fuel selection, materials handling, training, and fuel switching;
- coal and mineral round robin services: ensuring quality laboratory results and procedures;
- stockpile inventory services: determining the quantity and quality of coal and coke in storage; and
- other environmental services.

Two firms dominate the market for coal testing: Commercial Testing and Engineering Company (CT&E), headquartered in Lombard, IL, and Standard Laboratories (SL) of South Charleston, WV. CT&E is a wholly owned subsidiary of SGS North America, Inc., the North American division of the world's largest inspection and testing company, Société Générale de Surveillance (SGS). As shown in Table C-3, CT&E had revenues of $57.0 million in 1997 and employed 600 professionals at more than 50 locations in the contiguous U.S. SL's revenues were $37.0 million in 1996. SL employs approximately 500 people at more than 50 locations in the U.S. and abroad. Both companies together control over 90 percent of the contractual coal testing market (Vaninetti, 1998).

Most of the laboratories owned by SL and CT&E are located either in coal-producing states or at main ports for imported and export coal (see Figure C-2). Laboratories are primarily concentrated in key coal areas, mainly West Virginia, Kentucky, Colorado, and Wyoming. Coastal laboratories analyze samples for the coal import-export market. For example, CT&E's San Pedro, CA, facility serves the ports of Long Beach, Los Angeles, and San Francisco. The Norfolk, VA, facility serves the ports of Norfolk Southern Coal,

Table C-3. Sales and Employment of Major Coal Testing Laboratories

Two companies, CT&E and SL, dominate the market for coal testing services.

Company	Revenue ($million)[a]	Employment[a]	Location
Commercial Testing & Engineering	$57	600	Lombard, Illinois
Parent: SGS North America	$400	5,900	Parsippany, New Jersey
Ultimate Parent: SGS S.A.	$2,260[b]	28,000	Geneva, Switzerland
Standard Laboratories	$37	500	South Charleston, West Virginia

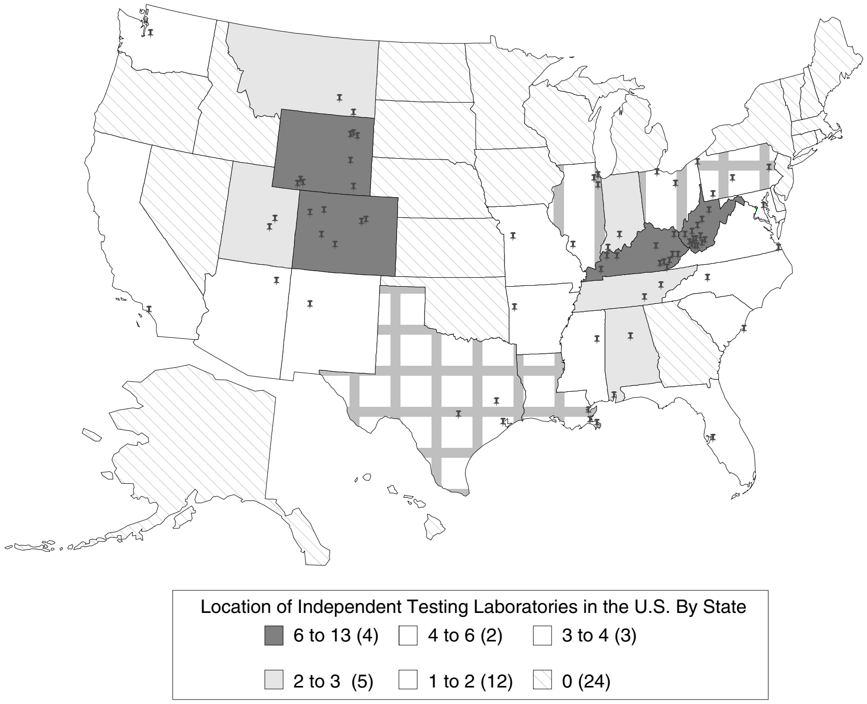
[a] Revenue and employment data for CT&E are for 1997. Revenue and employment for SL are for 1996.

[b] At current exchange rate (1.44 CHF/$).

Source: Information Access Company. 1998. Business Index [computer file]. Foster City, CA: Information Access Corporation.
Société Générale de Surveillance Holding S.A. 1988. *1997 Annual Report.* Geneva: Société Générale de Surveillance S.A.

Figure C-2. Location of Independent Coal Testing Laboratories in the U.S.

Most of the laboratories owned by CT&E and SL are located either in coal-producing states or at main ports for imported and exported coal.



Source: Commercial Testing & Engineering Company. 1998. "Sampling Services." As obtained on December 2, 1998. <http://www.comteco.com/sampleserv.htm>.
Standard Laboratories (SL). 1998. "Contract Laboratory Services—Standard Labs—Coal Test." As obtained on December 2, 1998. <http://www.coaltest.com/CONTLABS.htm>.

Morehead City, Richmond, Baltimore, and New York, among others. Other CT&E coastal lab cities include Charleston, Tampa, Toledo, Tukwila (Seattle), Mobile, and Deer Park (Houston).

These companies also operate contract test laboratories on-site for the mining industry. SL operates 30 such laboratories in the U.S. and abroad (SL, 1998). When mines have on-site laboratories, it is usually to test the coal for their coal preparation plants. Utilities may have in-house laboratories to test sulfur, heating value, moisture, and ash to ensure proper equipment operations, regulatory compliance, and/or blending operations.

Oil companies routinely operate their own laboratories that conduct product testing, including sulfur content testing, on petroleum products. Unlike the coal industry, the oil industry is more vertically integrated, with companies owning exploration firms, pipelines, refineries, and testing laboratories. However, independent testing laboratories for petroleum products are becoming more important. Table C-4 shows the primary independent petroleum testing laboratories in the U.S. Functioning similarly to coal laboratories, independent testing laboratories specializing in oil testing conduct tests on petroleum products and waste oils for contractual purposes and as a part of larger consulting projects. Firms providing petroleum testing services are concentrated in states with large refinery capacity, such as Texas, New Jersey, Oklahoma, and California.

C.1.2 Fossil Fuel Extraction and Processing

The combustion of fossil fuels supplies the majority of energy used by the residential, commercial, and industrial sectors. As shown in Figure C-3, in 1997 fossil fuels, including coal, petroleum products, and natural gas, supplied 85 percent of U.S. energy consumption. The U.S. is a net importer of energy products, with petroleum products being the largest energy import. Coal is the largest source of domestic energy production, accounting for 32 percent of domestic Btu production.

Table C-5 provides energy consumption by sector. After processing and refining, approximately two-thirds of fossil fuels are used directly to produce heat and work. The remainder is used by power plants to generate electricity that is subsequently used to generate heat and work.

Table C-4. Sales and Employment of Petroleum Testing Laboratories
The 24 companies listed below test for sulfur in petroleum products.

Company	Company Revenue ($million)	Employment[a]
Alpha Analytical Labs., Inc.	0.75	12
American Interplex Corp.	4[a]	NA
American Testing and Research, Inc.	1.75	19
Analysts, Inc.	15[a]	NA
Analytical Service Consultants	0.3	NA
Aspen Research Corp.	15	120
Atlantic Petroleum Services, Inc.	1.75	20
Bennett Testing Service, Inc.	1	7
Camin Cargo Control, Inc.	5.75	120
Conam Inspection Inc.	43.1[a]	725
Core Laboratories (Saybolt, Inc.)	92.3[b]	NA
Dallas Laboratories, Inc.	0.3	5
Harris Testing Laboratories, Inc.	0.3	7
Hydrocarbon Technologies Analytical Lab, Inc.	0.75	7
Inspectorate America Corp.	60[b]	600
Intertek Testing Services	85[b]	800
King Laboratories, Inc.	0.75	7
Martel Laboratories JDS, Inc.	3.75	40
Oil Science Laboratory	0.3	1
Oiltest, Inc.	2.5	51
Paragon Laboratories, Inc.	0.75	9
Quanterra Incorporated	41.7[b]	800
Saybolt Inc.	35	NA
SGS Control Services, Inc. (NA)	61.5[b]	720

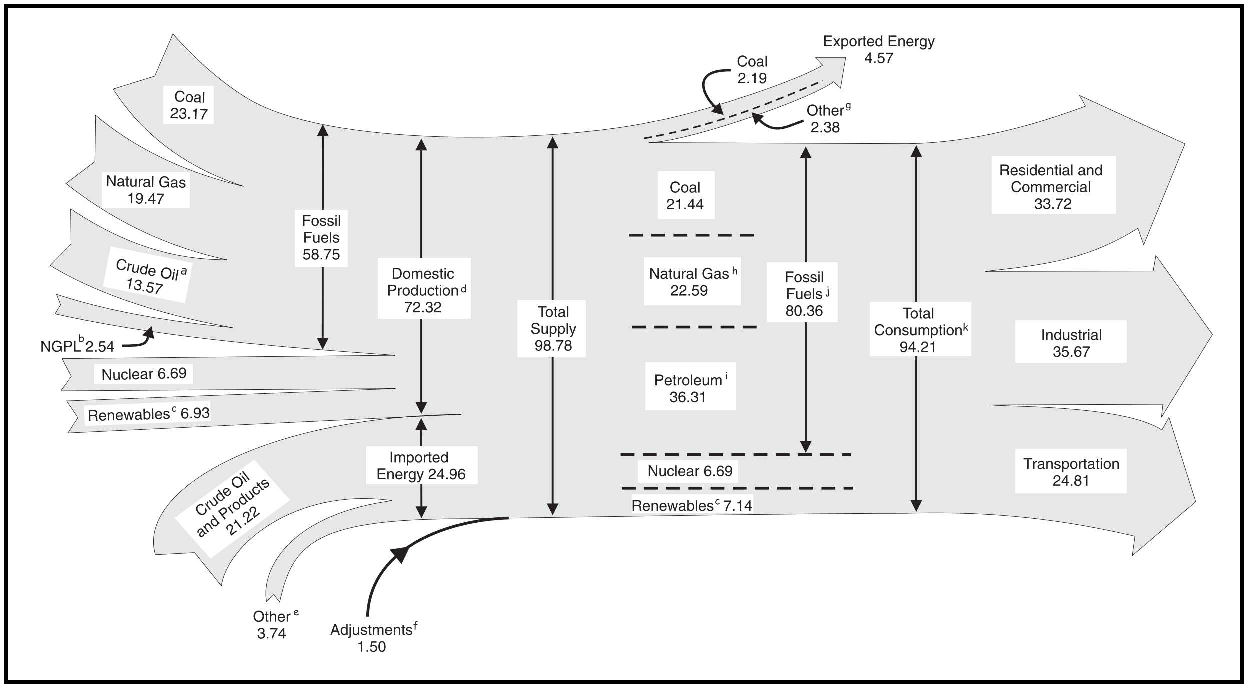
[a] Information Access Company. 1998. Business Index [computer file]. Foster City, CA: Information Access Corporation.

[b] Dun & Bradstreet, 1999. *D&B Million Dollar Directory: America's Leading Public and Private Companies.* Bethlehem, PA: Dun & Bradstreet, Inc.

Source: American Society for Testing and Measurement. 1999. *1999 Directory of Testing Laboratories.* <http://www.astm.org/labs/>. As obtained on February 16, 1999.
Company Data Source: American Business Information, Inc. 1998. The American Business Disk [computer file]. Omaha, NE: American Business Information.

Figure C-3. Energy Flow, 1997 (quadrillion Btu)

Fossil fuels supply about 85 percent of U.S. energy consumption.



[a] Includes lease condensate.

[b] Natural gas plant liquids.

[c] Biofuels, conventional hydroelectric power, geothermal energy, solar energy, and wind energy.

[d] Includes –0.04 quadrillion Btu hydroelectric pumped storage.

[e] Natural gas, coal, coal coke, and electricity.

[f] Stock changes, losses, gains, miscellaneous blending components, and unaccounted for supply.

[g] Crude oil, petroleum products, natural gas, electricity, and coal coke.

[h] Includes supplemental gaseous fuels.

[i] Petroleum products, including natural gas, plant liquids, and crude oil consumed directly as fuel.

[j] Includes 0.02 quadrillion Btu coal coke imports.

[k] Includes, in quadrillion Btu, 0.16 net imported electricity from nonrenewable sources; -0.04 hydroelectric pumped storage; and –0.10 ethanol blended into motor gasoline, which is accounted for in both fossil fuels and renewables.

Notes: Data are preliminary. Totals may not equal sum of components due to independent rounding.

Source: U.S. Department of Energy, Energy Information Administration. 1998a. *Annual Energy Review 1997*. DOE/EIA-0384(97). Washington, DC: Department of Energy. Tables 1.1, 1.2, 1.3, 1.4, and 2.1.

Table C-5. End-Use Energy Consumption, 1996 (quadrillion Btu)
Energy consumption is roughly equally divided among residential and commercial, industrial, and transportation uses.

Sector	Gas	Coal	Petroleum Products	Electricity[a]	Other (Coke, Breeze, Biofuels, Net Steam, and Raw Materials)	Losses[b]	Total
Residential and Commercial	8.63	0.14	2.18	7.04	0.72	14.98	33.69
Industrial	10.39	2.42	9.07	3.52	2.63	7.48	35.51
Transportation	—	—	23.89	—	1.00	—	24.89
Total	19.02	2.56	35.14	10.56	4.35	22.46	94.09

[a] Electricity generation: 50.5 percent coal, 15.3 percent gas, 1.9 percent oil, and 32.3 percent nonfossil fuel (nuclear, hydroelectric, and renewables).

[b] Total losses are calculated as the sum of energy consumed at electric utilities to generate electricity, utility purchases of electricity from nonutility power producers, and imported electricity, minus exported electricity and electricity consumed by end users. Total losses are allocated to the end-use sectors in proportion to each sector's share of total electricity use.

Source: U.S. Department of Energy, Energy Information Administration. 1998a. *Annual Energy Review, 1997.* Washington, DC: Department of Energy.

The industries accounting for the majority of fossil fuel combustion are electrical power, petroleum, iron and steel, and trucking.

The industries accounting for the majority of fossil fuel combustion are electrical power, petroleum, iron and steel, and trucking. As shown in Table C-6, power plants use approximately 90 percent of coal to generate electricity. The trucking industry consumes approximately 65 percent of all petroleum products used in the U.S. in the form of diesel fuel.[4]

National trends in coal consumption are an environmental concern because the combustion of coal is a major source of sulfur released to air. Table C-7 shows the trend of coal consumption from 1992 to 1997. The consumption of coal by electric utilities increased from 1992 to 1997. However, coal consumption by electric utilities is expected to decrease as new gas-fired generation units are bought online and older coal units are retired.

Coal Industry

The U.S. coal industry produces and distributes 1.1. billion short tons of coal per year. The industry consists of a few very large companies that produce more than 5 percent of total coal production and many mid-size and small companies. Information about the sulfur content of coal is very important to this industry

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[4] The trucking industry accounts for approximately 78 percent of freight bills, and fuel expenditures represent a large share of the trucking industry's expenditures.

Table C-6. Fossil Fuel Combustion by Industry and Sector

Approximately 90 percent of coal is used by power plants to generate electricity.

Industry	Coal (thousand short tons, 1996)	Coal (%)	Oil (thousand barrels, 1996)[a]	Oil (%)	Natural Gas (thousand cubic feet, 1995)	Natural Gas (%)
Electricity Generation	874,681	88.9%	116,800	1.75%	3.2	16.2%
Iron and Steel (and Coke)	31,706	3.2%	6,680[b]	0.10%	0.5a	2.5%
Petroleum Refining	—	—	12,050[b]	0.18%	0.7a	3.5%
Industrial Combustion	70,941	7.2%	1,757,870	26.30%	7.4	37.6%
Transportation	—	—	4,372,700	65.42%	0	0.00%
Commercial and Other	6,006	0.6%	427,050	6.39%	3.0	15.2%
Residential	0	0.0%			4.9	24.9%
Total	983,334	100%	6,683,150	100%	19.7	100%

[a] All liquid fossil fuels, including fuel oils, diesel fuel, and gasoline.

[b] 1994 amounts.

Sources: Coal data from U.S. Department of Energy, Energy Information Administration. 1998a. *Annual Energy Review, 1997*. Washington, DC: Department of Energy.
National Mining Association. "Coal Statistics, 1992-1997." <http://www.nma.org/coalstats.html>. As obtained on November 18, 1998.
U.S. Department of Energy, Energy Information Administration. 1998a. *Annual Energy Review, 1997*. Washington, DC: Department of Energy.

Table C-7. Coal Consumption, 1992 to 1997 (thousand short tons)

The consumption of coal by electric utilities has increased since 1992 but is expected to decrease in the near future.

	1992	1993	1994	1995	1996	1997
Total Consumption	892,421	925,944	930,201	940,880	983,334	1,007,813
Electric Utilities	779,830	813,508	817,270	829,007	874,681	907,662
Coking	32,366	31,323	31,740	33,011	31,706	29,443
Other Industrial	74,042	74,892	75,179	73,055	70,941	70,702
Residential/Commercial	6,153	6,221	6,013	5,807	6,006	6,006

Source: National Mining Association. "Coal Statistics, 1992-1997." <http://www.nma.org/coalstats.html>. As obtained on November 18, 1998.

because the price of coal is a function of its sulfur content among other attributes. Removing sulfur from coal is expensive, and the sulfur content of coal determines whether an electric utility plant that burns it can meet its regulatory emissions requirements for SO_2.

Characteristics of Coal Supply. The U.S. Department of Energy's Energy Information Administration (EIA) estimates U.S. recoverable reserves of coal to be over 270 billion short tons of varying sulfur content. U.S. annual coal production has been increasing steadily since the mid-1990s despite a 34 percent drop in the number of mines. Table C-8 presents selected coal supply statistics for 1992 to 1997. Between 1992 and 1997 coal production increased more than 9 percent to nearly 1.1 billion short tons. Western coal, which is generally lowest in sulfur content, accounted for most of the growth, with a 30 percent increase in production. Cost-cutting measures and the abandonment of small mines brought the number of mines in the U.S. down from 2,746 in 1992 to 1,810 in 1997.

Table C-8. Selected Coal Supply Statistics, 1992 to 1997

U.S. coal production increased by 9 percent during the mid-1990s despite a 34 percent drop in the number of mines.

	1992	1993	1994	1995	1996	1997
Production (thousand short tons)	997,545	945,424	1,033,504	1,032,974	1,063,856	1,089,932
Appalachian	456,565	409,718	445,370	434,861	451,868	464,737
Interior	195,659	167,174	179,858	168,526	172,848	172,290
Western	345,321	368,532	408,276	429,587	439,140	451,592
Value of Production at Mine ($1,000)	$20,978,371	$18,766,666	$20,060,312	$19,450,900	$19,681,336	$19,801,979
Price Indicators (avg. $/short ton)						
Value at Mines	$21.03	$19.85	$19.41	$18.83	$18.50	$18.19
Cost at Electric Utility	$29.36	$28.58	$28.03	$27.01	$26.45	$26.16
Number of Mines	2,746	2,475	2,354	2,104	1,903	1,810
Underground	1,354	1,196	1,143	977	885	810
Surface	1,392	1,279	1,211	1,127	1,018	1,000

Source: U.S. Department of Energy, Energy Information Administration. 1998f. *Coal Industry Annual, 1997.* Washington, DC: U.S. Department of Energy.

The composition of coal varies greatly across fields. The key properties of coal are its relative levels of carbon, hydrogen, moisture content, heating value, and sulfur. The heating value of a coal determines its "rank." The rank of a particular coal is determined largely by the fixed (or nonvolatile) carbon content. Coals are ranked as follows from lowest to highest: lignite, subbituminous, bituminous, and anthracite.

Other characteristics of coal, aside from heating value, also vary by rank. Tables C-9 and C-10 summarize some of the key characteristics of coal of different rankings. The value of coal is primarily a function of its Btu content and moisture content. However, sulfur content also influences the value of coal. Coal contains up to 10 percent sulfur (by weight), which is released during burning and oxidizes to SO_2 or sulfate (SO_4) in the atmosphere.

Table C-9. Composition and Heating Value of "As-Received" Coals
Anthracite and bituminous coals have the highest commercial value because of their high heating value and low moisture content.

	Composition (weight percentage)				
Rank	Moisture	Volatile Matter	Fixed Carbon	Ash	Heating Value (Btu/lb)
Anthracite	3-6	4-12	75-85	4-15	12,000-13,500
Bituminous	2-15	15-45	50-70	4-18	12,000-14,500
Subbituminous	10-25	30-45	31-55	3-12	8,000-11,000
Lignite	35-45	22-32	25-30	4-15	6,000-7,500

Source: Glasstone, Samuel. 1980. "Energy Deskbook." National Technical Information Services, U.S. Department of Commerce. DE82013966 (DOE/IR/05114-1).

Table C-10. Chemical Composition of Coals by Type (Moisture and Ash Free)
The sulfur content of coal ranges from 0.2 to 6 weight percent.

	Weight Percentage				
Rank	Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
Anthracite	75-85	1.5-3.5	5.5-9	0.5-1.0	0.5-2.5
Bituminous	65-80	4.5-6.0	4.5-10	0.5-2.5	0.5-6.0
Subbituminous	57-69	5.5-6.5	15-30	0.8-1.5	0.2-2.0
Lignite	35-45	6.0-7.5	38-48	0.5-1.0	0.3-3.0

Source: Glasstone, Samuel. 1980. "Energy Deskbook." National Technical Information Services, U.S. Department of Commerce. DE82013966 (DOE/IR/05114-1).

Of the three primary types of fossil fuels, coal has the highest sulfur content by percent weight and heat content. It contains up to 10 percent sulfur (by weight).

Coal is generally classified into four sulfur categories: compliance, low sulfur, medium sulfur, and high sulfur. Compliance coal has the lowest sulfur content of 0.6 pounds per million Btus or less. It naturally falls within federal emissions regulations and therefore requires less cleaning before combustion. Low-sulfur coal has between 0.61 and 1.25 pounds of sulfur per million Btus, medium sulfur coal between 1.26 and 1.67 pounds per million Btus, and high-sulfur coal more than 1.67 pounds per million Btus.

Coal's sulfur content varies by the location from which it is mined. Generally, western coal (from Colorado, North Dakota, and Wyoming, for example) is lowest in sulfur; Appalachian coal (from Pennsylvania, West Virginia, and Kentucky, for example) is either low or medium sulfur; and interior coal (from Indiana, Illinois, Ohio, for example) is medium and high sulfur.

Many variables affect the price of coal. The price a utility pays per short ton of coal is a function of quantity purchased, heating value, sulfur and ash content, distance from the mine, and the supplier's costs. Coal from surface mines is less expensive than coal from underground mines because surface mines operate using less capital and labor, all other things held equal. For a utility, the prices paid for coals of varying sulfur content may differ significantly precisely because so many factors affect prices (see Table C-11). A utility may pay a higher price for higher-sulfur content coal because that coal has a greater healthy value than a lower-sulfur content coal. All other things held equal, however, high-sulfur coal is less expensive than low-sulfur coal.

Coal Industry Structure. The coal industry consists of a few large companies and many smaller companies. In 1997, the U.S. had over 1,800 coal mines employing about 83,000 people (EIA, 1997). Table C-12 lists the top 40 coal producers in the U.S in 1996. The largest coal producer, Peabody Holding Co., Inc., produces 13.4 percent of total U.S. coal production. The top four companies generate about 33 percent of total production; the top ten companies produce about 51 percent, and the top 20 produce about 66 percent (EIA, 1997). Many companies that own coal mines are engaged primarily in another industry that requires a large quantity of coal. For example, many power companies produce coal, as do Aluminum Company of America and General Dynamics Corporation.

Table C-11. Average Delivered Cost of Coal by Sulfur Content and Region for Electric Utilities, 1997 ($ per short ton)

The price a utility pays per short ton is a function of quantity purchased, sulfur and ash content, distance from mine, and the supplier's costs.

		Sulfur Content					
Region	**Average**	**0.5% or Less**	**More than 0.5% up to 1.0%**	**More than 1.0% up to 1.5%**	**More than 1.5% up to 2.0%**	**More than 2.0% up to 3.0%**	**More than 3.0%**
New England	43.67	50.10	43.25	43.74	43.36	40.44	—
Middle Atlantic	34.39	16.93	39.56	36.40	33.78	32.21	35.94
East North Central	27.68	23.54	33.45	30.30	29.82	25.80	29.26
West North Central	15.39	15.71	13.48	18.04	30.99	24.69	28.36
South Atlantic	36.34	26.83	38.58	37.58	33.21	37.52	27.62
East South Central	28.70	22.74	37.46	29.76	32.03	25.65	21.27
West South Central	19.69	23.12	13.58	12.42	9.49	26.32	14.10
Mountain	21.52	21.21	21.79	15.83	—	—	—
Pacific Contiguous	25.19	21.11	26.33	—	—	—	—
Pacific Noncontiguous	—	—	—	—	—	—	—
Total	**26.16**	**21.18**	**29.16**	**28.86**	**30.57**	**28.53**	**27.35**

Note: Figures may not add to total because of independent rounding.

Source: U.S. Department of Energy, Energy Information Administration. 1998b. *Cost and Quality of Fuels for Electric Utility Plants 1997 Tables*. Washington, DC: U.S. Department of Energy.

Coal Processing Technology. Coal processing entails the mining, cleaning, and distribution of coal from underground and surface mines. Figure C-4 provides an overview of activities, inputs, and outputs of the coal processing industry.

Coal is extracted from two categories of mines: underground and surface mines. Underground coal mining entails cutting a slot, known as a kerf, at the bottom of a face; drilling holes in the face for explosives or compressed air; blasting the coal; and loading and hauling it out of the working area to a conveyor belt or mine cars. (Pennsylvania Department of Environmental Protection, 1999). Surface mining refers to the removal of dirt and rock on top of a coal seam so that it can be excavated, placed on conveyors, and sent to preparation plants. Strip mining is the most popular surface mining method in the U.S.

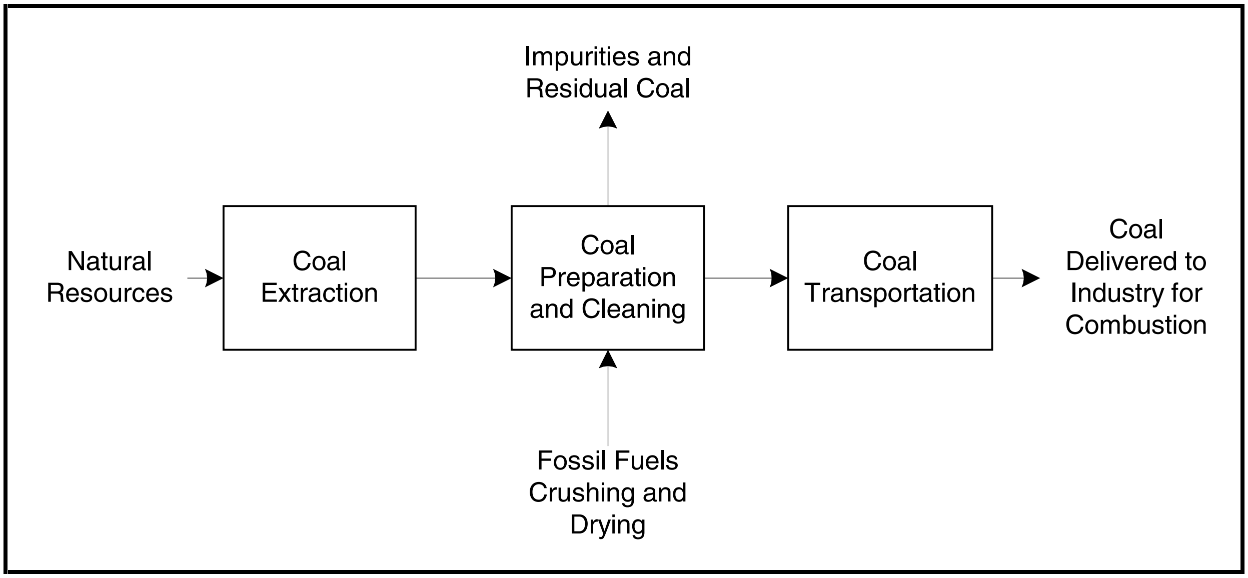
Table C-12. Top Forty U.S. Coal Producers, 1996

While the largest coal producer controls a large percentage of the market, the coal market has many mid-size and small producers.

Company Name	Production (thousand short tons)	Percentage of Total Production	Cumulative Percentage
Peabody Holding Co., Inc.	142,811	13.4	13.4
Cyprus AMAX Minerals Co.	74,738	7.0	20.4
Consol Energy Inc.	70,072	6.6	27.0
Kennecott Energy Co.	62,527	5.9	32.9
ARCO Coal Co.	51,013	4.8	37.7
Kerr-McGee Coal Corp.	31,350	2.9	40.6
Zeigler Coal Holding Co.	31,001	2.9	43.5
Marrowbone Development Co.	29,239	2.7	46.2
Texas Utilities Co.	28,214	2.6	48.8
A.T. Massey Coal Co.	27,327	2.6	51.4
North American Coal Corp.	26,284	2.5	53.9
Arch Mineral Corp.	30,153	1.9	55.8
Montana Power Co.	19,623	1.8	57.6
Ashland Coal Inc.	16,091	1.5	59.1
Marigold Land Co.	14,731	1.4	60.5
Pittston Coal Group	13,281	1.2	61.7
BHP Utah Minerals	13,228	1.2	62.9
Pittsburg & Midway Coal Mining Co.	19,246	1.2	64.1
Mapco Coal Inc.	12,844	1.2	65.3
Kiewit Coal Properties, Inc.	9,863	0.9	66.1
Costain Coal Inc.	9,342	0.9	67.0
The Coastal Corp.	8,932	0.8	67.8
AEP Service Corp.	8,652	0.8	68.6
Jamer River Coal Co.	8,025	0.8	69.4
Andalex Resources Inc.	7,613	0.7	70.1
Drummond Company Inc.	7,342	0.7	70.8
Rochester & Pittsburgh Coal Co.	7,315	0.7	71.5
Jim Walter Resources Inc.	7,313	0.7	72.2
U.S. Steele Mining Co., Inc.	7,169	0.7	72.9
Black Beauty Coal Co.	6,628	0.6	73.5
Teco Coal Corp.	6,615	0.6	74.1
Aluminum Company of America	8,379	0.5	74.6
Westmoreland Resources Inc.	5,111	0.5	75.1
General Dynamics Corp.	4,741	0.4	75.5
Ohio Valley Resources Inc.	4,538	0.4	75.9
Minnesota Power & Light	4,199	0.4	76.3
Hanson PLC	4,132	0.4	76.7
Lee Ranch Coal Co.	3,828	0.4	77.1
Exxon Corp.	3,689	0.3	77.4
Sun Co., Inc.	3,554	0.3	77.7

Source: U.S. Department of Energy, Energy Information Administration. 1997. *Coal Industry Annual, 1996.* Washington, DC: U.S. Department of Energy.

Figure C-4. Coal Processing
Coal preparation and cleaning are used to remove sulfur and other impurities.



On-site coal preparation plants make coal more valuable through size reduction, desulfurization, and removal of moisture and inorganic impurities. Nearly 50 percent of the coal mined in the U.S. passes through coal preparation plants; east of the Mississippi River this number increases to 80 percent (Fonseca, 1995). Coal preparations, which "clean" coal by removing impurities, may account for 5 to 15 percent of the cost of coal production (Horton and Bloom, 1993).

Coal preparation plants remove coal mechanically by taking advantage of differences between the impurities and the coal's density. Water is used to fluidize a bed of crushed coal and its contaminants. As the lighter coal particles float to the top, the impurities are separated. The coal is then skimmed off the top of the bed and dried using a combination of hot gases. Coal is also blended to meet customer specifications. For example, high- and low-sulfur coal may be mixed together as part of the preparation and cleaning process to ensure the sulfur content of the delivered coal meets sulfur levels specified in contracts.

Petroleum Refining

The U.S. petroleum industry supplies over 6 billion barrels of petroleum products per year. The industry is dominated by a small number of large, vertically integrated companies. This structure is driven by the large capital costs associated with the petroleum refining technology. Sulfur information allows refineries to control the sulfur content of output streams and emissions. Both are required for regulatory compliance.

Characteristics of Petroleum Supply. The value of crude oil is a function of its elemental composition, which determines the type and grade of the final product it can be used to produce. The hydrocarbons present in petroleum release a significant amount of heat upon combustion and are the major determinant of petroleum's heating value (measured in Btu/gal or Btu/barrel). Table C-13 contains the elemental composition ranges of typical crude oils.

Table C-13. Approximate Elemental Composition Ranges of Most Petroleum Oils

Sulfur content in crude oil typically ranges from 1 to 2 percent. However, some crude oil has up to 6 percent sulfur.

Element	Weight Percentage
Carbon	82 to 87
Hydrogen	11 to 15
Nitrogen	Up to about 1
Oxygen	Up to about 2
Sulfur	Up to about 6
Metals	Up to about 0.05

Source: Glasstone, Samuel. 1980. "Energy Deskbook." National Technical Information Services, U.S. Department of Commerce. DE82013966 (DOE/IR/05114-1).

The sulfur found in crude petroleum is removed from refined products by a process known as hydrodesulfurization. The resulting hydrogen sulfide must then be removed from stack gasses to prevent its release to the environment.

Petroleum is commonly classified according to its specific gravity or by its API gravity.[5] These are both measures of density. A lower specific gravity is equivalent to a higher value on the API scale. Most crude petroleum oils have specific gravities in the range of 0.80 to 0.95, which corresponds to 45 to 17 degree API. Lower specific gravity (higher API) is typically linked to a higher market value.

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[5] API gravity is an arbitrary scale expressing the gravity or density of liquid petroleum products. The higher the API gravity, the lighter the compound. Light crudes generally exceed 38 degrees API and heavy crudes are commonly labeled as crudes with API gravity of 22 or below. Intermediate crudes fall into the range of 22 to 38 API gravity.

The sulfur content is an important characteristic of crude oil. The composition of crude oil varies greatly from field to field throughout the world. For example, Alaskan crude typically has a low sulfur content (sweet), and South American crude typically has a high sulfur content (sour). Crude oil with a high sulfur content is more expensive to refine because it is difficult to separate sulfur compounds from pure hydrogen/carbon compounds (Leffler, 1985). As shown in Table C-14 the main determinants of crude oil prices are sulfur content (sweet versus sour) and API gravity (light versus heavy). High API gravity, or light crude, is more valuable because it is used in more high-end products when distilled and has fewer impurities.

Table C-14. Prices and Sulfur Content for Selected Crude Streams
Crude oil prices depend on both API and sulfur content.

Crude Stream	Price (average 1997) ($/barrel)	Sulfur (weight percentage)	API
Nigrerian Bonny Light	21.21	0.13	35.4
UK Brent	20.85	0.35	37.4
Gaben Rabi-Kouanga	20.07	0.05	34.3
Mexican Olmeca	20.02	0.72	39.1
Angolan Cabinda	19.48	0.17	32.0
West Texas Intermediate	19.27	0.3	39.1
Venezuelan Furrial	18.59	1.16	27.4
Saudi Arabian Light	18.14	1.1	38.4
West Texas Sour	17.77	1.65	34.1
Saudi Arabian Medium	17.11	2.5	30.1
Canadian Bow River Heavy	16.46	2.1	24.7
California Wilmington	16.44	1.7	16.9
Mexican Mayan	15.58	3.43	22.2
Alaskan North Slope	14.84	1.0	27.0

Sources: U.S. Department of Energy, Energy Information Administration. Petroleum Marketing Monthly. 1998e. Haverly/Chevron Assay Library. <http://www.haverly.com.chevfram.htm>.

Table C-15 lists the net production of petroleum products in 1997. Almost 90 percent of the products generated by petroleum refining are used as fuels (gasoline, diesel and distillate fuel oil, liquefied petroleum gas, jet fuel, residual fuel oil, kerosene, and coke). The

Table C-15. Production of Petroleum Products
Most refinery products are used as fuels such as motor gasoline and distillate fuel oil.

Commodity	U.S. Annual Production (thousand barrels)
Liquefied Refinery Gases	252,168
Finished Motor Gasoline	2,826,051
Finished Aviation Gasoline	7,248
Jet Fuel	567,295
Kerosene	23,887
Distillate Fuel Oil	1,238,041
0.05 percent sulfur and under	789,287
Greater than 0.05 percent sulfur	448,754
Residual Fuel Oil	258,290
Less than 0.31 percent sulfur	26,090
0.31 to 1.00 percent sulfur	75,334
Greater than 1.00 percent sulfur	156,866
Naphtha for Petrochemical Feedstock Use	83,569
Other Oils for Petrochemical Feedstock Use	79,539
Special Naphthas	19,191
Lubricants	8,372
Waxes	251,619
Petroleum Coke	84,294
Asphalt and Road Oil	177,019
Still Gas	241,184
Miscellaneous Products	17,501
Total	6,116,870

Source: U.S. Department of Energy, Energy Information Administration. 1998c. *Petroleum Supply Annual,* Volume 1. Washington, DC: U.S. Department of Energy.

remaining 10 percent include finished nonfuel products (solvents, lubricating oils, greases, petroleum wax, petroleum jelly, asphalt, and coke) and chemical industry feedstocks (naphtha, ethane, propane, butane, ethylene, propylene, butylenes, butadiene, benzene, toluene, and xylene). Chemical feedstocks are used as a primary input to a number of products, including fertilizers, pesticides, paints, waxes, thinners, solvents, cleaning fluids, detergents, refrigerants, antifreeze, resins, sealants, insulations, latex, rubber compounds, and plastics.

Petroleum Industry Structure. In the U.S., most crude oil distillation capacity is owned by large integrated companies (EPA, 1995). Until recently, the petroleum refining industry was categorized as oligopolistic because it was dominated by the top four firms in the industry. Over 30 percent of the market share was attributable to these four firms: Exxon Corp., Mobil Corp., El du Pont de Nemours and Co., and Texaco Inc. However, the market concentration ratios for these top firms have been marginally decreasing in recent years (EPA, 1995). The large companies generally have the greatest control over residual fuel sales, while distillate sales have been decreasing for these companies in recent years.

Petroleum Processing Technology. Petroleum refining is the physical, thermal, and chemical separation of crude oil into its major distillation fractions, which are then further processed through a series of separation and conversion steps into finished petroleum products and chemical industry feedstocks. The primary input to the refining process is crude oil, which accounts for 92 percent of input feed.

Four primary categories of operations are implemented at a petroleum refinery:

- the desalting process;
- separation processes, which are used to divide crude oil into its major components;
- conversion processes, which involve restructuring petroleum molecules to convert crude oil components into gasolines and other light fractions; and
- petroleum treating processes, which serve the purpose of stabilizing and upgrading petroleum products by separating them from less desirable products and removing undesirable elements such as sulfur (EPA, 1995).

Sulfur is removed from petroleum products by reacting it with hydrogen gas in the presence of a catalyst at a moderately high temperature and pressure. This process is referred to as hydrodesulfurization or hydrofinishing. In addition to desulfurization of final products, sulfur recovery for sale of elemental sulfur is also conducted for refinery process off-gas streams as part of emissions reduction activities. The sulfur is converted to hydrogen sulfide, which is then absorbed through desulfurization of stack gases.

Desulfurization of petroleum output streams can be very expensive. As part of background research for the development of its new sulfur content in gasoline regulations, EPA developed estimates of the cost of removing sulfur from gasoline. As shown in Table C-16, reducing the sulfur content of gasoline from its pre-Tier-2 levels (about 330 ppm) to 40 ppm is about 1.6 cents per gallon.

Table C-16. Cost of Reducing the Sulfur Content of Gasoline from its Current Level (about 350 ppm) to Alternative Levels

As the sulfur content of gasoline is reduced, the incremental cost of removing each additional ppm of sulfur increases.

Sulfur Level	EPA Estimate of Cost per Gallon (cents)	API Estimate of Cost per Gallon (cents)
150 ppm	0.7	2.3 to 2.6
100 ppm	1.1	
40 ppm	1.6	
30 ppm	1.7	

Source: U.S. Environmental Protection Agency. April 1999. *Draft RIA for Control of Air Pollution from New Motor Vehicles: Tier 2 Motor Vehicle Emissions Standards and Gasoline Sulfur Control Requirements.*

The American Petroleum Institute (API) believes that EPA underestimated the added cost of reducing the sulfur content of gasoline below current levels. The trade association funded a series of studies conducted by MathPro that estimated the cost to be 2.3 to 2.6 cents per gallon (*Octane Week*, 1999). Although API's estimates are listed in Table C-16, the economic estimates presented in this study are based on the more conservative EPA estimates of approximately 1 cent per gallon.

> The varying content of sulfur in crude oil makes it difficult to maintain specific sulfur levels in output streams.

Maintaining specific sulfur levels in output streams and process off-gas streams is difficult because of the varying content of sulfur in crude oil. Accurate information about the sulfur content of the crude oil and the output streams is essential to maintaining product specifications and maximizing the efficiency of the processing equipment.

Frequently, refineries specialize in crude streams with either high or low sulfur content. Because desulfurization equipment is expensive, a company's high-sulfur crude refining will typically be concentrated in a few large facilities to increase equipment utilization and decrease costs. Large refineries are generally more flexible compared to small refineries in their ability to substitute one type of crude oil input for another.

Coke Industry

Coke is metallurgical coal that has been baked into a charcoal-like substance. This substance burns more evenly and at a higher temperature compared to coal. Coke is primarily used as an input for producing steel in blast furnaces at integrated iron and steel mills (i.e., furnace coke) and as an input for gray, ductile, and malleable iron castings in cupolas at iron foundries (i.e., foundry coke). Therefore, the demand for coke is a derived demand that is largely dependent on production of steel and iron castings.

The sulfur content of coke affects the quality of iron and steel, the cost of production, and the cost of environmental compliance.

The sulfur content of coke affects the production process and the sulfur content of iron and steel and that industry's regulatory compliance. Low-sulfur iron and steel is more valuable than high-sulfur iron and steel. Furthermore, the lower the sulfur content of coke, the lower the emissions of sulfur compounds during the iron and steel production process. Coke's sulfur content is primarily determined by the sulfur content of the coals used to produce it. Alternatively, additional steps can be added to the production process to reduce the amount of sulfur in coke. However, these processes add to the cost of production; thus, facilities generally prefer to use lower-sulfur coals to avoid additional desulfurization processes (Zaino and Brousseau, 1983).

Characteristics of the Coke Industry. The manufacture of coke is included under Standard Industrial Classification (SIC) code 3312—Blast Furnaces and Steel Mills. However, coke production is a small fraction of this industry.

Table C-17 summarizes coke industry capacity and production by type of producer and type of coke. There are two primary types of coke producers: integrated producers and merchant producers. Integrated producers, which manufacture about 79 percent of all coke, are owned by steel companies. Merchant producers, which manufacture the remaining 21 percent of coke, sell their product to steel manufacturers.

In 1997, the coke industry produced about 20 million short tons of coke. About 90 percent of that coke was furnace coke to be used in blast furnaces for steel making. The remaining 10 percent was

Table C-17. Summary of Coke Operations at U.S. Companies, 1997

Most furnace coke is produced by integrated producers, while foundry coke is supplied by merchant producers.

Company Name	Number of Coke Plants	Total Coke Capacity (short tons/yr)	Coke Production by Type (short tons/yr)			
			Furnace	Foundry	Other	Total
Integrated Producers						
Acme Metals Inc.	1	500,000	493,552	0	19,988	513,540
AK Steel Corp.	2	1,429,901	1,352,986	0	0	1,352,986
Bethlehem Steel Corp.	2	2,627,000	2,420,387	0	82,848	2,503,235
Geneva Steel Co.	1	800,000	700,002	0	16,320	716,322
HMK Enterprises Inc.[a]	1	500,000	521,000	0	0	521,000
LTV Corp.	2	1,164,000	1,133,406	0	0	1,133,406
National Steel Corp.	2	1,526,701	1,479,387	0	0	1,479,387
USX Corp.	2	7,823,045	6,667,594	0	0	6,667,594
WHX Corp.[b]	1	1,247,000	1,249,501	0	36,247	1,285,748
Total Integrated Producers	14	17,617,647	16,017,815	0	155,403	16,173,218
Merchant Producers						
Aloe Holding Co.[c]	1	514,779	354,137	0	0	354,137
Citizens Gas and Coke	1	634,931	173,470	367,798	93,936	635,204
Drummond Co. Inc.[d]	1	699,967	25,806	727,720	0	753,526
Erie Coke Corp.	1	214,951	0	122,139	19,013	141,152
Koppers Industries Inc.	1	372,581	358,105	0	0	358,105
McWane Inc.[e]	1	162,039	0	142,872	0	142,872
New Boston Coke Corp.	1	346,126	317,777	0	0	317,777
Sun Co. Inc.[f]	2	1,949,000	649,000	0	0	649,000
Tonawanda Coke Corp.	1	268,964	207,234	136,225	63,822	407,281
Walter Industries[g]	1	451,948	268,304	131,270	33,500	433,074
Total Merchant Producers	11	5,615,286	2,353,833	1,628,024	210,271	4,192,128
Total	25	23,232,933	18,371,648	1,628,024	365,674	20,365,346

[a] Owns Gulf States Steel, Inc.

[b] Owns Wheeling-Pittsburgh Corp.

[c] Owns Shenango Inc.

[d] Owns ABC Coke.

[e] Owns Empire Coke.

[f] Owns Indiana Harbor Coke Co. and Jewell Coke and Coal Co.

[g] Owns Sloss Industries Corp.

Sources: U.S. Environmental Protection Agency. 1998c. *Coke Industry Responses to Information Collection Request (ICR) Survey*. Database prepared for EPA's Office of Air Quality Planning and Standards. Research Triangle Park, NC. Association of Iron and Steel Engineers (AISE). 1998. "1998 Directory of Iron and Steel Plants: Volume 1 Plants and Facilities." Pittsburgh, PA: AISE.

foundry coke to be used for making iron castings. About 89 percent of furnace coke was manufactured by integrated iron and steel facilities.

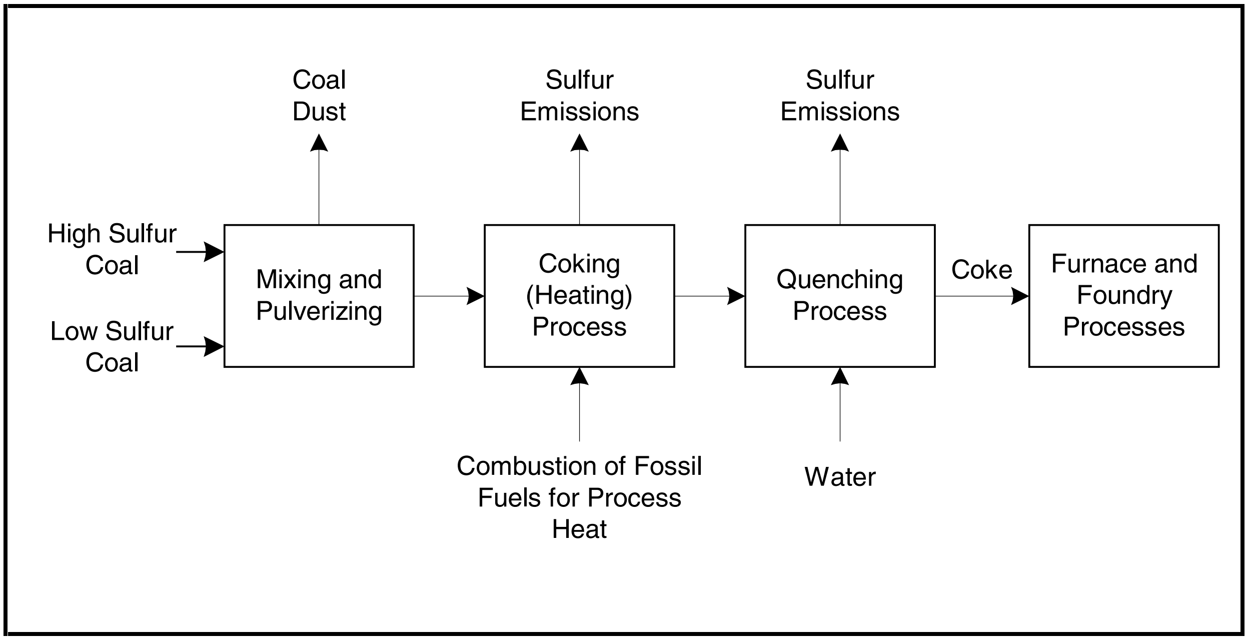
Table C-17 lists the coke-producing companies in the U.S. Nineteen companies own a total of 25 coke plants in the U.S. The nine integrated producers own 14 coke plants, while the ten merchant produces own 11 coke plants. Captive consumption currently dominates the U.S. furnace coke market. Integrated producers account for about 87 percent of all furnace coke. In 1997, six companies produced foundry coke in the U.S. The U.S. foundry coke market is fairly concentrated, with two companies currently accounting for two-thirds of U.S. production—Drummond Co. Inc., with 45 percent, and Citizens Gas and Coke, with 22.6 percent. The remaining four merchant producers each account for between 7.5 and 8.8 percent of the market.

Coke Manufacturing Process. Coke is produced by heating pulverized coal at high temperatures in large ovens without oxygen for 14 to 36 hours and then cooling it with a water spray.

Figure C-5 presents the inputs, production activity, major emissions, and product outputs for the industry.

Figure C-5. Coke Production

Sulfur emissions occur during both the coking process and the quenching process.



Metallurgical coal is delivered to coke manufacturing plants in railroad cars or barges. It is then transferred to mixing bins where the various types of coal are blended based on specific characteristics of the coal such as fluidity, ash, and sulfur content. Lankford et al. (1985) consider the selection of coals to be the single most important factor in establishing coke quality. The best coals are low in ash and sulfur content and produce a structurally strong coke. Coal blending results in improved and more consistent coke quality, which justifies the extra expense of mixing.

Coke production involves three basic steps:
- ➤ mixing and pulverizing
- ➤ coking
- ➤ quenching

The coal is pulverized and fed into the oven. The coal in the coke oven is heated at temperatures up to 2,000 ºF for 14 to 36 hours. When subjected to such a high degree of heat in the absence of air, the chemical compounds making up coal are unstable and the complex organic molecules break down to yield gases and a relatively nonvolatile carbonaceous residue (i.e., coke). At the end of the coking cycle, doors on each end of the oven are removed, and the incandescent coke is pushed from the oven.

During what is known as the wet quenching process, the incandescent coke is carried to a quench tower where it is cooled to a temperature of 200 º to 500 ºF by a system of stationary water sprays and air dried in preparation for sizing. This quenching prevents the coke from burning up in the air. The coke is then screened to a uniform size, which also results in some small coke fines (or breeze) that are recovered for use as a raw material input to blast furnaces.

C.1.3 Fuel Combustion

As explained earlier in Appendix C, the primary uses of fossil fuels in the U.S. are the production of power by electric utilities, the production of steel, and the production of power by industrial boilers. This section describes the structure of the electric power industry and the steel industry. However, we do not address industrial combustion. Because industrial boilers are used in all major industrial sectors, it would be very difficult for us to characterize this diverse set of industries.

Electricity Generation

Approximately 35 percent of all U.S. fossil fuel consumption (measured in Btus) is used to generate electricity. Electricity generation in 1996 consumed 88.9 percent of coal, 1.7 percent of oil, and 16.2 percent of natural gas used in the U.S. Because of its dependence on coal as a fuel, electricity generation accounts for 65.9 percent of SO_2 released into the atmosphere. The electric generation industry is heavily regulated because it is one of the primary sources of SO_2 emissions in the U.S.

The electric utility industry relies heavily on sulfur content information to determine fuel mix and other operating parameters that affect its compliance with environmental regulations. Furthermore, many power plants are designed to burn coal of a specific sulfur content. Burning high-sulfur coal in these plants can lead to boiler fouling and slagging, decreased generating efficiency, and increased maintenance costs.

Characteristics of the Electricity Generation Industry. Electric utilities produce 88 percent of electricity generated in the U.S. Electric utilities are typically large publicly owned entities whose primary function is to generate and distribute electricity. Nonutility generators account for the remaining 12 percent of electricity generation and are comprised mainly of independent power producers and industrial facilities engaged in self-generation and cogeneration. Cogeneration refers to the combined production of electricity with another form of useful energy, such as process heat or steam.

The electric utility industry is very dependent on fossil fuels, especially coal. Fossil fuels account for over two-thirds of net megawatthours (MWh) generated in the U.S. (EPA, 1998c). As shown in Table C-18, nuclear, hydroelectric, renewable, and other fuels account for the remaining net generation. Within the fossil fuel category, coal is used as the main energy source to generate electricity in the utility industry, and natural gas is the main energy source for nonutility generators. Other fossil fuels used much less frequently to generate electricity are petroleum coke, refinery gas, coke oven gas, blast furnace gas, and liquefied petroleum gas. Future trends are for natural gas to increase its share of both utility and nonutility electricity generation because of rapid technology improvements in combined-cycle gas turbine engines.

Table C-18. Net Generation by Energy Source, 1996
Although most new generating units built during the past few years are gas-fired units, coal units still account for over half of electricity generation in the U.S.

Energy Source	Utility Generators (million kWh)	Nonutility Generators[a] (million kWh)	Total (million kWh)
Fossil Fuels			
Coal	1,737,453	61,424	1,798,877
Natural Gas	262,730	213,359	476,089
Petroleum	67,346	14,951	82,297
Nuclear	674,729	—	674,729
Renewable			
Hydroelectric	331,058	16,555	347,613
Geothermal	5,234	10,198	15,432
Biomass	1,967	57,997	59,964
Other	13	4,303	4,316
Other	—	3,744	3,744
Total	3,080,530	382,531	3,463,061

[a] Gross generation: Approximately 60 percent of electricity produced by nonutility generators is sold to electric utilities.

Source: U.S. Department of Energy, Energy Information Administration. 1998d. *Electric Power Annual*, Volumes I & 2. Washington, DC: U.S. Department of Energy.

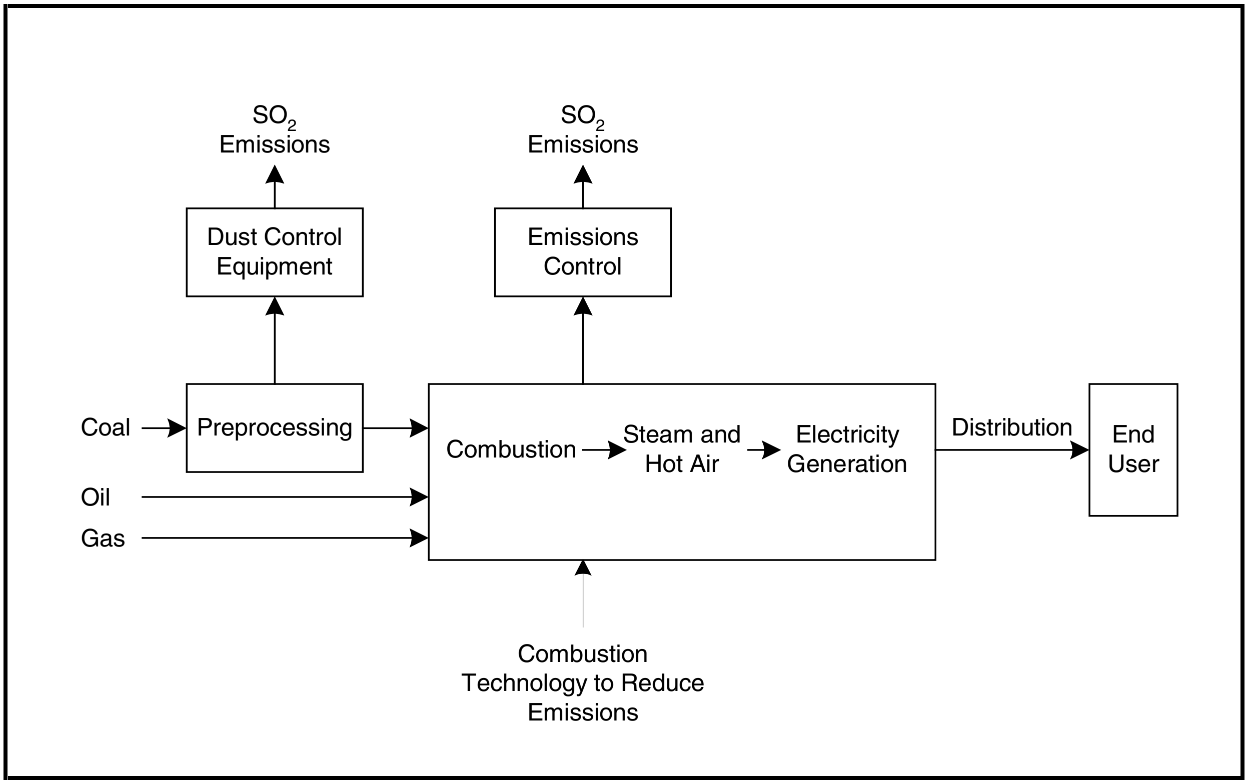
Electricity Generation Process. Figure C-6 shows an overview of the electricity generation process using fossil fuel. Through controlled combustion, the Btu potential in fossil fuels is converted into either steam or hot air, which is then used to generate electricity.

Several generation technologies are commonly used to produce electricity, including boilers to fire steam turbines, gas turbines, internal combustion engines, and combined-cycle generation. Combined-cycle generation produces electricity by passing one source of hot gas through two separate thermal cycles, thereby increasing efficiency by reducing waste heat.

The sulfur content of coal affects the performance of electricity generating equipment, the amount of preprocessing required, and the level of emissions control required to achieve compliance.

The sulfur content of the coal determines, in part, the extent of the processing required prior to combustion. Coal can be cleaned and prepared to reduce sulfur content. The cleaning of coal also increases its fuel efficiency (effective Btu content). However, cleaning coal is a costly process and is more efficiently conducted at the mine by using gravity concentration, flotation, or dewatering methods. Accurate sulfur information is used to determine the amount of precleaning and postcleaning activities required to comply with environmental regulations.

Figure C-6. Electricity Generation Process
Sulfur emissions occur during coal preprocessing and fuel combustion.



Most petroleum used for electricity generation is refined prior to use and shipped to the generating plant by pipeline. The fuel oils most commonly used for electricity generation include fuel oil numbers 4, 5, and 6 (heavy oil).

Steel Industry

The U.S. iron and steel industry (including coke) consumes approximately 3.2 percent of the U.S. coal supply. In addition, the iron and steel industry accounts for 2.5 percent of natural gas and 0.1 percent of oil consumption (EIA, 1998a). Most coal is converted into coke prior to use in the steel manufacturing process.

The steel industry uses sulfur information primarily to control product quality and also to ensure environmental compliance. There is an inverse relationship between sulfur levels and steel quality. Low-sulfur steels (<0.010 percent sulfur) have greater ductility and better impact properties than steels with high sulfur content. Low-sulfur steels are demanded by vehicle manufacturers and pipe manufacturers because of their impact and corrosion resistance, which enhances the quality of end-use products (Zaino and Brousseau, 1983).

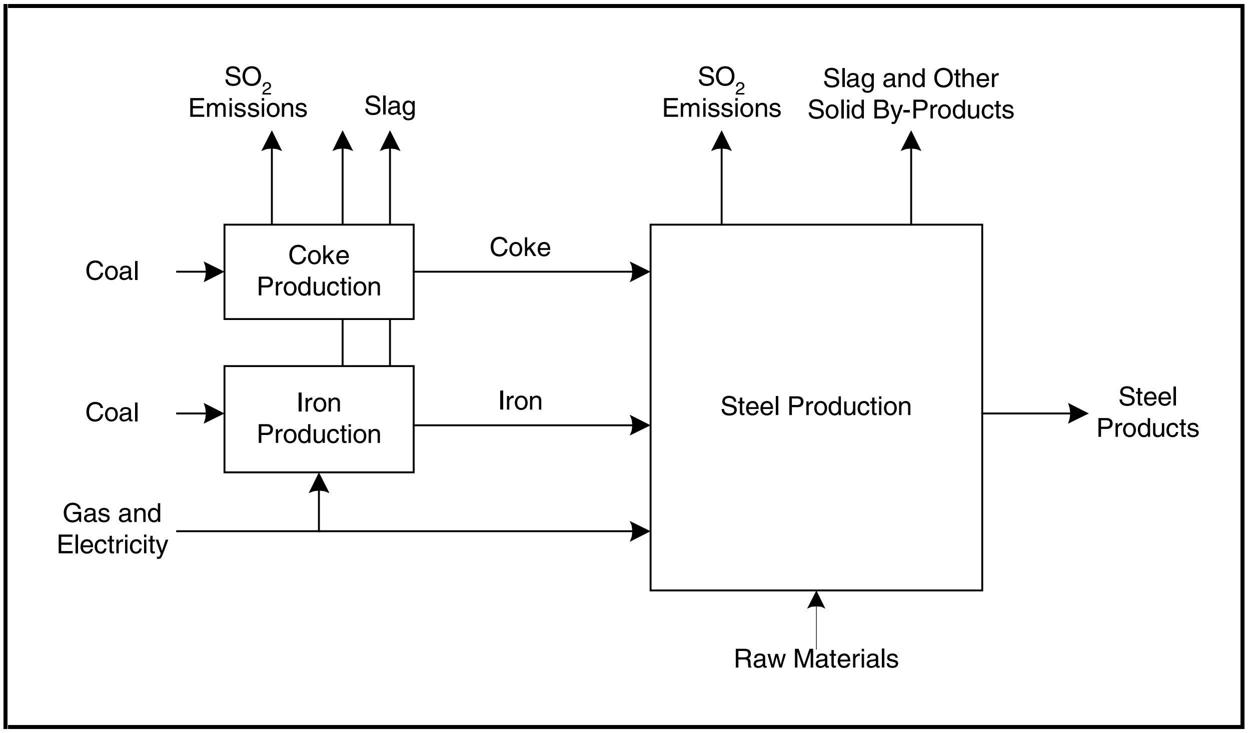
Characteristics of the Steel Industry. The U.S. iron and steel industry can be separated into three distinct types of producers: integrated mills, nonintegrated or specialty mills, and mini-mills. Integrated iron and steel producers are companies that produce iron from iron ore in blast furnaces. The integrated producers in the U.S. are listed in Table C-17. Their principal commercial activity is the production and sale of carbon steel. Integrated producers use furnace coke in blast furnaces and either produce coke on site or purchase it from merchant coke producers. Nonintegrated or specialty mills do not have the necessary equipment to produce steel from basic raw materials; instead, they purchase these inputs in a processed form (i.e., semi-finished products) to manufacture steel products. Mini-mills use only electric arc furnaces (EAFs) to melt scrap steel and other materials to make steel products.

From 1980 to 1990, integrated iron and steel production in the U.S. decreased approximately 60 percent. This decline was due to slow growth in demand for steel, markets lost to substitute materials, increased foreign competition, and low productivity growth resulting from older and less-efficient capital stock. However, while the integrated producers were contracting, the mini-mills were more than doubling their capacity and expanding into new markets. As a whole, the U.S. steel industry experienced a turnaround in 1993 with shipments at their highest level since 1981. This increase was due to the strong demand from the automotive and construction industries and the weak dollar (making imports more expensive). As of 1997, integrated producers accounted for roughly 55 percent of U.S. steel production, with 20 plants operating at a total steel capacity of almost 6.2 million short tons per year (AISI, 1998; EPA, 1998a).

In 1994, iron and steel facilities consumed 1,907 trillion Btus of energy. The vast majority of this energy, 1,119 trillion Btus, was in the form of coke and breeze. Natural gas and electricity supply most of the industry's remaining energy needs.

Manufacturing Process. Steel facilities manufacture steel by melting, alloying, and molding pig iron and steel scrap. Figure C-7

Figure C-7. Integrated Iron and Steel Production
Sulfur emissions are generated during coke production and steel production.



presents the inputs, production activity, major emissions, and product outputs for the industry.

Raw materials used in the production process include molten or pig iron (iron that is allowed to cool and solidify), iron and steel scrap, foundry returns, metal turnings, alloys, carbon additives, sand, sand additives, binders, and fluxes. Fluxes are materials that are added to collect impurities from the metal, such as carbon compounds. The most widely used flux is lime; other fluxes include soda ash, fluorspar, and calcium carbide. Iron is manufactured by combining iron ore, coke, and flux and heating the mixture at high temperatures.

The steel-making process generally consists of combining and melting ingredients before pouring the liquid steel into molds to be packed and cooled. Scrap metals are cleaned and degreased with solvents prior to being mixed with pig iron. Typically the metals are melted in large EAFs or basic oxygen furnaces. When the melting process is complete, the molten metal is poured directly into molds.

C.2 THE IMPORTANCE OF SULFUR IN FOSSIL FUELS

This section describes the regulatory and technical issues that make the sulfur content of fossil fuels important. The sulfur content of a fuel is important for two reasons: because sulfur has a detrimental effect on the environment and because sulfur content can affect the performance of a product or process. For both reasons, the sulfur content of fossil fuels affects its value; thus, information about sulfur content is essential to trade and production.

C.2.1 Environmental Regulation of Sulfur in Fossil Fuels

Sulfur's detrimental impact on the environment has led to regulations of the sulfur content of fossil fuels and the sulfur emissions of facilities burning fossil fuels. Because sulfur is expensive to remove, these regulations have resulted in a price premium for low-sulfur-content fossil fuels.

Because some sulfur compounds have a detrimental effect on human health, wildlife, agricultural productivity, and quality of life, sulfur compound emissions from some sources and sulfur content of some fuels are regulated by EPA and by state regulatory agencies. These regulations have evolved over time and have become more strict with respect to both sulfur content and sulfur compound emissions. We expect that this trend will continue, as EPA requires greater control over sulfur compound emissions and lower sulfur content in fossil fuels.

The primary environmental concern is sulfur dioxide (SO_2), which is produced from the combustion of fuels that contain sulfur as an impurity. Sulfur dioxide is directly harmful to health when inhaled and indirectly harmful because it generates acid rain.

Table C-19 shows the share of SO_2 emissions by fossil fuel type. Because of coal's chemical composition, typically containing 2 to 6 weight percent sulfur, the mining, processing, transportation, and combustion of coal account for 80 percent of domestic fossil fuel SO_2 emissions. In contrast, the combustion of natural gas, which has a much lower Btu-to-sulfur ratio, generates approximately 4 percent of total domestic SO_2 emissions.

Table C-20 lists SO_2 emissions for the major industries directly affected by environmental regulation. Electricity generation, through its high consumption of coal, is the major generator of SO_2 emissions, accounting for about two-thirds of these emissions. Industrial combustion, primarily in industrial boilers, accounts for approximately 18 percent of SO_2 emissions. Reductions in

Table C-19. Sulfur Dioxide Emissions by Fossil Fuel Type (thousand short tons)
The mining, processing, transportation, and combustion of coal account for 80 percent of domestic fossil fuel SO_2 emissions.

Fuel	SO_2 (%)
Coal	80.1
Oil	15.8
Natural Gas	4.1
Total	100

Source: U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards. December 1997b. *National Air Pollution Emissions Trends, 1990-1996*. Research Triangle Park, NC: U.S. Environmental Protection Agency.

Table C-20. Sulfur Dioxide Emissions by Industry, 1996 (thousand short tons)
Electricity generation is responsible for about two-thirds of SO_2 emissions.

Industry	SO_2	SO_2 (%)
Electricity Generation	12,604	65.9
Iron and Steel (coke)	151	0.8
Petroleum Refining	271	1.4
Petroleum Production	89	0.5
Industrial Combustion	3,399	17.8
Others	2,599	13.4
Total	19,113	100

Note: Totals may not sum due to independent rounding.

Source: U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards. December 1997b. *National Air Pollution Emissions Trends, 1990-1996*. Research Triangle Park, NC: U.S. Environmental Protection Agency.

emissions from power generation and ferrous metals processing are projected to reduce the total amount of SO_2 emissions from coal consumption over the next decade. The projected reduction is due, in part, to expected reductions in the use of coal by electric utilities as new gas-fired generation units are brought on line and older coal units are retired.

Regulations that control the emissions of sulfur to the environment fall under two broad types: sulfur content regulations and sulfur emissions regulations. Both types of regulations are supported by standards that control the way in which sulfur content and sulfur emissions are tested.

Sulfur Content Regulations

The Clean Air Act of 1970 authorized EPA to regulate product quality through specific formulations of gasoline and other fuels. The main national programs currently regulating sulfur content in fossil fuels are the National Highway Diesel Fuel Program and the National Ambient Air Quality Standards (NAAQS). The highway diesel fuel program required that the sulfur content of all highway diesel fuel be reduced from 0.5 percent (5,000 ppm) to 0.05 percent (500 ppm) by October 1, 1993. California limits the sulfur content of diesel fuel to between 300 and 500 ppm. Reducing SO_2 emissions from gasoline was one of the primary goals included in the 1971 NAAQS. In addition, other provisions of the Act limited the sulfur content in residual and distillate fuel oils used by electric utilities and industrial plants.

Currently, the sulfur content of fuels used by industry and EPA for federal vehicle certification can differ substantially from gasoline actually sold nationwide. Because the emissions performance of LEVs is sensitive to the sulfur content of fossil fuels, these vehicles do not perform as well on the road with high-sulfur fuels as they do during testing.

New federal regulation promulgated under the Clean Air Act will limit the sulfur content of gasoline by 2004. The federal legislation, formally proposed in May 1999, is known as "Tier 2" Emissions Standards for Vehicles. It is based on actions taken by California to reduce motor vehicle emissions to improve air quality. Because low sulfur content of gasoline supports advanced emissions control technologies, California restricts the sulfur content of gasoline to no more than 40 ppm or, alternatively, to a quarterly average of 30 ppm with a cap of 80 ppm (EPA, 1998b). Federal regulations to be phased in by 2004 will set similar sulfur content levels for all gasoline sold in the U.S. Current and emerging sulfur content regulations are an indirect result of efforts to limit automobile emissions of SO_2 as well as other pollutants.

This legislation was prompted, in part, by tremendous progress in technology to reduce emissions from gasoline-fueled vehicles. The emissions performance of these low emissions vehicles (LEVs) is very sensitive to the sulfur content of gasoline. Emissions control technology is often designed to meet the vehicle emission standards of California, which currently has the most stringent vehicle emission standards in the world. The vehicles are also designed to run on the low-sulfur content gasoline sold in California. While gasoline in California averages less than 30 ppm and is limited to no more than 80 ppm, gasoline in the U.S. outside of California currently averages over 330 ppm and can reach levels as high as 1,000 ppm (EPA, 1998b). This high sulfur level can significantly reduce catalyst performance and increase the emissions of these vehicles. Low-sulfur gasoline is needed to enable the use of advanced emissions control technologies.

For these reasons, there was increasing momentum toward federal sulfur content regulation. In November 1997, the American Automobile Manufacturers Association (AAMA) and the Association of International Automobile Manufactures (AIAM) petitioned EPA to establish a national, year-round limit on gasoline sulfur. Their request echoed California's sulfur content limits. In California, the sulfur content of gasoline must not exceed 40 ppm on an annual average of 30 ppm. In addition, an individual gallon of gasoline must not exceed 80 ppm. This request was based not only on its immediate impact on the industry's ability to meet emissions requirements, but also on its importance for accommodating the newest generation of automobile catalysts for LEVs and other new vehicle technologies.

The new Tier 2 emissions standards make California emissions the national standard. Beginning in 2004, all cars and light trucks sold in the U.S., including sport utility vehicles, minivans, and pickup trucks, will be equipped with advanced emissions control technologies. The impact of these technologies and low-sulfur gasoline will allow vehicles to be 77 to 95 percent cleaner than they are today (EPA, 1999).

BP Amoco recently announced that it will begin selling low-sulfur gasoline in 40 cities worldwide. Currently, BP Amoco's *Amoco Ultimate* gasoline has the industry's lowest sulfur content (outside of California) at 200 ppm. BP Amoco's goal is to meet or exceed the 2005 European goal of 50 ppm (*News and Observer*, 1999).

Regulation of Sulfur Emissions

EPA regulates air emissions of SO_2 from a variety of sources to reduce adverse health and environmental effects. Under the 1990 Clean Air Act Amendments, EPA developed national emissions standards for 186 hazardous chemicals, including SO_2 and sulfur oxide (SO_X). National emissions standards for hazardous air pollutants (NESHAPs) regulations specify an emissions limit based on what is achievable with a specific control technology and the chemical content of the inputs to the production process. For example, to achieve the limits, petroleum refineries using crude oils with different levels of sulfur content may require different scrubber technologies on the catalytic cracker's gas flue.

As a criteria pollutant, SO_2 (combined with other sulfur oxides as SO_X) is also regulated under new source review (NSR) and new source performance standards (NSPSs). NSR requirements are typically conducted by state agencies. This program applies to new facilities or expansion of existing facilities or process modifications and requires facilities to meet lower achievable emission rate (LAER) standards compared to existing (unchanged) facilities. SO_2 also falls under NAAQS and the acid rain program.

These emissions regulations affect all industries that use fossil fuels as a fuel input, including petroleum refineries, coke and steel plants, utility boilers, and industrial boilers.

These regulations affect industries' fuel choices and profitability. For example, public utilities commissions (PUCs) may have to approve utilities' fuel switching and emissions technology choices, and they define the way costs are treated in the rate base and how electricity prices are established (Bohi, 1994). Emissions reductions have typically been achieved by specifying pollution control technologies for SO_2 emissions sources.

Air emissions from the stack gases from coal- and oil-fired boilers are primarily regulated through technology-based performance standards included in state and local permits. These performance standards commonly identify specific combustion technologies or end-of-pipe scrubber equipment that can be applied to individual units (referred to as sources) to demonstrate compliance. These technologies may require coals of a specific sulfur content (EPA, 1997a).

In addition to technology-based performance standards, generating units may also be subject to other local or regional environmental regulations, including NAAQ standards, the Acid Rain Program, and the Acid Rain Allowance Trading Program.

NAAQ standards do not directly affect the fossil fuel electric power generation industry because they are not applied to individual sources. Rather, these standards are applied to the ambient air in a particular area. Fossil fuel electric generators may be indirectly affected by these standards if they are located in or near an area with nonattainment status. Generators in nonattainment areas may be targeted for more stringent controls implemented through local operating permits.

The *Acid Rain Program* was authorized by the Clean Air Act to reduce the adverse effects of acidic deposition on natural resources, ecosystems, materials, visibility, and public health. The principal sources of acidic compounds are emissions of SO_2 and NO_x from the combustion of fossil fuels. To support the mandated reductions in SO_2 and NO_x, EPA issued regulations requiring facilities in acid rain regions to install continuous emission monitoring systems (CEMS). In addition, all generating units in these regions over 25 megawatts (and new units under 25 megawatts) that use fuel with sulfur content greater than 0.05 percent by weight are required to measure and report emissions under the Acid Rain Program (EPA, 1997a).

The Acid Rain Allowance Trading Program is an innovative approach included in the 1990 Clean Air Act Amendments intended to reduce the costs of compliance while meeting the same (or improved) environmental objectives. The approach provides a firm with the flexibility to find the most cost-effective way of achieving compliance through trading SO_2 allowances. The trading system exploits the potential efficiency gain from equating the marginal cost of abatement (pollution reduction) for individual sources within a facility and across companies in a trading region (RFF, 1996). In the year 2001, steelmakers will join electric utilities in trading SO_2 emissions allowances under Title IV of the Clean Air Act Amendments of 1990.

Individuals can be fined up to $25,000 per day for violations and can be sentenced to a year in prison. Corporations can be fined up to $1,000,000 for each offense.

The market price for SO_2 allowances is one measure of the impact of sulfur content on the value of fossil fuels. The allowance price is primarily determined by the market availability of low-sulfur coal and the cost of purchasing and operating emissions abatement technologies, such as SO_2 scrubbers. In June 1998, the market price for SO_2 allowances hit a record high of $190 per ton (ACA, 1998).

For facilities exceeding emissions limits (whether or not they are inadvertent), enforcement agencies can bring legal action resulting in fines, prison terms, or both. Individuals can be fined up to $25,000 per day for violations and can be sentenced to a year in prison. Corporations can be fined up to $1,000,000 for each offense. Furthermore, repeat offenders can have fines and sentences doubled.

Other remedies exist for facilities that cannot meet an emissions limitation. Production rates can be reduced to reduce emissions, or agreements can be established with permitting agencies to allow full production in exchange for emissions reductions in other processes or for other actions acceptable to the agencies.

C.2.2 Sulfur's Role in Product and Process Quality

In addition to its detrimental impact on the environment, sulfur content also affects the quality of products and processes that use fossil fuels. For example, catalysts for low-emissions vehicles are sensitive to the sulfur content of gasoline and diesel fuel. Similarly, the catalysts used in petroleum processing can be "poisoned" by sulfur; sulfur affects the technical quality of other petroleum products as well. Fuel oils used in heat-treating metals or in firing glass-melting furnaces must be low in sulfur to avoid damaging the product. The sulfur content of coke has an impact on the quality of the steel it is used to produce. As explained below, these technical issues elevate the importance of accuracy and precision in the measurement of sulfur content.

Sulfur Impact on Vehicle Catalysts

The technology for the low emissions vehicles of the future requires low-sulfur fuels to operate efficiently. Sulfur in gasoline increases exhaust emissions by decreasing the efficiency of the catalysts used in current and advanced emissions control systems. The sulfur affects the precious metals used in the catalyst; palladium is especially sensitive to sulfur poisoning. Similarly, metal oxides used to manage the oxygen concentrations in the exhaust are also affected by sulfur (*Hart's Fuel Technology & Management's Sulfur 2000*, 1998).

Sulfur in gasoline can also have a detrimental effect on emerging engine technologies. For example, the gasoline direct-injection (GDI) engine offers the promise of improved fuel economy, improved engine response under variable operating conditions, and more rapid starting. However, performance of this technology is sensitive to the sulfur content of gasoline. New fuel cell technologies are also sensitive to the sulfur content of gasoline.

Sulfur in Other Petroleum-Based Products and in Refinery Processing

Other petroleum-based products are sensitive to the presence of sulfur compounds. For example, undesirable sulfur compounds in base oils used for lubricants lead to poor performance in lubricant products. However, sulfur is present in many of the additives blended into the base oils to enhance performance. Base oil, additive, and lubricant product specifications typically include allowable sulfur levels. Hence, monitoring sulfur levels for these products is key to quality control.

Fuel oils used in heat-treating metals or in firing glass-melting furnaces must be low in sulfur to avoid damaging the product. In addition, some expensive process catalysts used in petroleum and chemical refining can be poisoned when trace amounts of sulfur-bearing materials are contained in feedstocks.

Steel

Scientists have determined that one factor contributing to the demise of *The Titanic* was that the steel used in its construction had a high sulfur content, which caused it to be brittle, especially under very cold conditions (Modern Marvels, 1999).

Sulfur is an undesirable property in steel except for special purposes. Sulfur with iron forms sulfide, which is soluble in the liquid metal and has a melting point lower than the other constituents of the iron. This phenomenon, called "hot-shortness," may cause weaknesses in the steel. Sulfur also increases the shrinkage of the iron, increasing the difficulty of making accurate castings, as well as the tendency to form cracks (which are a result of the high shrinkage) (Lankford et al., 1985). As a result, specifications for the maximum allowable sulfur content in various types of steel are on the order of 0.04 to 0.05 percent.

The major source of sulfur in the steel-making process is from coal, which is made into coke as described in Section C.1.2. Coal is processed into coke by a process called coking, which takes place in coke oven batteries. Coke that contains too much sulfur affects the productivity of the steel-making process as well as the sulfur content of the steel. Sulfur from the coke used in the blast furnace becomes part of the slag, which is a by-product of the blast furnace (the other product is molten iron). A good deal of the sulfur is removed from the blast furnace with the slag, which removes other impurities from the molten iron as well. If the coal contains too much sulfur, the volume of slag that is generated increases, decreasing the productivity of the blast furnace. Some sulfur remains dissolved in the iron (Lankford et al., 1985).

If the coal has too much sulfur, additional treatment is required to remove excess sulfur from the final product. After the iron is removed from the blast furnace, it goes through a desulfurization process. Flux materials are added to the iron, and the sulfur is removed in a ladle prior to charging the iron to the steel-making furnace (Lankford et al., 1985).

C.3 USAGE OF NIST SRMS IN THE FOSSIL FUEL INDUSTRY

As described in Section 3, NIST SRMs are used by the measurement and fossil fuel industries to develop CRMs, to calibrate instruments, and to check the accuracy of analytical methods. The chain of traceability of all sulfur measurements to NIST SRMs begins with the direct customers of NIST SRMS.

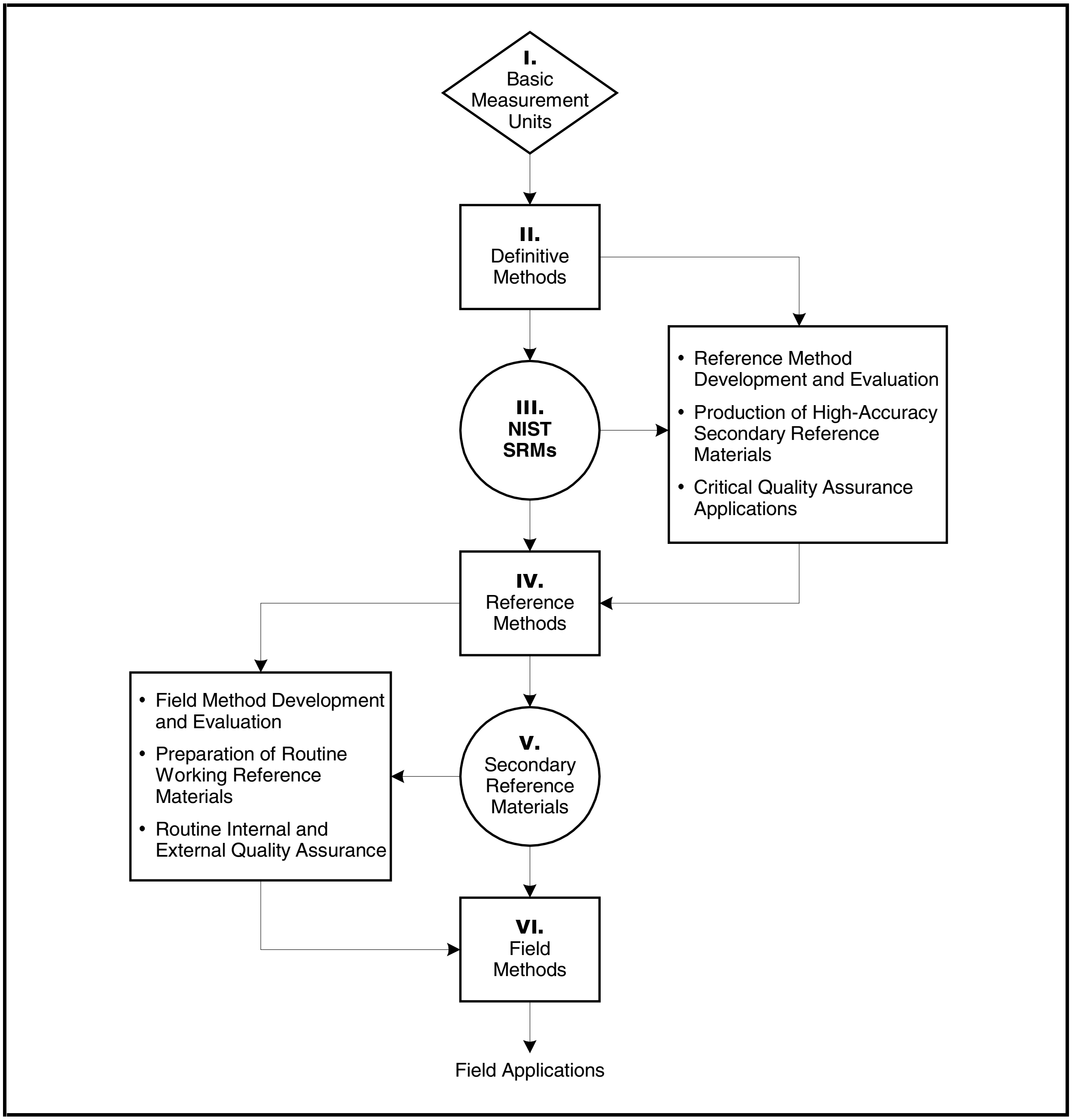
Figure C-8 shows the role that NIST SRMs play in the integrity of the measurement system. SRMs are developed using definitive methods that are tied to the basic measurement units maintained at NIST. NIST definitive methods are methods involving high precision primary techniques and have been critically evaluated for sources of bias in each specific application. SRMS are then used to develop and evaluate reference methods, to ensure the accuracy of secondary reference materials, and to ensue accuracy in critical quality assurance applications. Secondary reference materials and reference methods are then used to develop and evaluate field methods to prepare working reference material such as calibrants and to perform routine quality assurance activities. The integrity of this system is based on the quality of NIST SRMS and their traceability, through definitive methods, to the basic measurement units.

C.3.1 How Industry Uses NIST SRMs

SRMs play an integral role in users' quality control programs. Companies use SRMs in four ways: to calibrate equipment, to develop and validate the accuracy of analytical methods, to prepare

Figure C-8. SRM Role in Measurement Accuracy

NIST SRMs play an integral role in users' quality control programs. They are used to develop and evaluate analytical methods, to produce secondary standards, and in quality assurance applications.

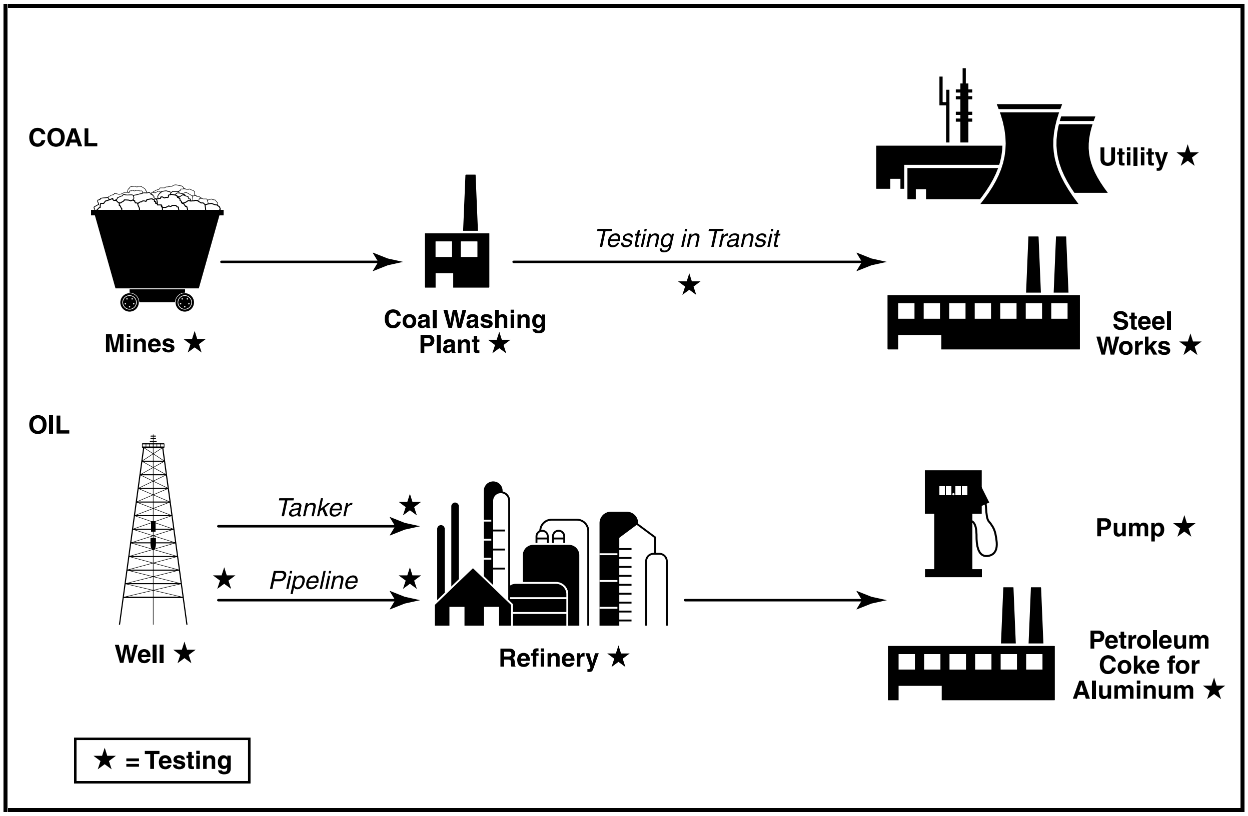


Source: Taylor, John K. 1993. *Standard Reference Materials: Handbook for SRM Users.* NIST Special Publication 260-100. Washington, DC: U.S Government Printing Office. February.

standards, and to set contracts and settle disputes. Figure C-9 illustrates the various points at which the sulfur content of the fuel may be tested.

Figure C-9. Sulfur Testing Along the Coal and Oil Supply Chain

Figure C-9 illustrates the various points at which the sulfur content of the fuel may be tested.



Because SRMs are costly, firms generally use NIST-traceable secondary reference materials for routine tasks. Companies' use of NIST SRMs is consistent with the model shown in Figure C-8. Generally, firms do not use SRMs each time they calibrate their equipment. Because SRMs are more costly than other reference materials, firms use NIST-traceable secondary reference materials to calibrate the equipment and perform other routine tasks. SRMs are used to verify that the equipment is properly calibrated. This technique allows firms to maintain traceability and quality while keeping costs down. NIST SRMs for calibration or calibration verification give users confidence in the precision of their instruments and the accuracy of those instruments' results.

Properly calibrated equipment is required for accurate sulfur-content testing and for applications development. Utilities, petroleum companies, coal companies, and other firms need properly calibrated equipment to ensure that the fuel they have bought or sold meets the sulfur-content specifications detailed in contracts. There are financial, and often regulatory, penalties for failing to meet those specifications. Equipment manufacturers use NIST SRMs to ensure that products are functioning properly and to test new prototypes.

NIST SRMs are also used in the production of certified reference materials, or CRMs. Many firms produce CRMs for in-house use or to sell to other firms and NIST SRMs are used in the quality control and production processes. By using NIST SRMs to calibrate equipment and validate equipment performance, CRM manufacturers make their products traceable to NIST. NIST traceability is a key component of a CRM manufacturer's credibility.

SRMs also support the analytical methods used by firms to take measurements and develop products and services. Indeed, many standard analytical methods call for SRMs because they are easily obtainable and authoritative. SRMs also allow firms to more accurately determine the bias of the methods they are using.

In addition, SRMs provide a common, independent benchmark from which industry can develop product specifications and legally binding contracts. Natural matrix SRMs are superior to other reference materials because they are certified using critically evaluated methods. SRMs lend credibility and legal defensibility to measurements.

When disputes over measurement accuracy arise between firms, SRMs are used as a referee material. For example, if a firm purchases a sulfur analyzer and later complains that instrument is not functioning properly, the manufacturer will validate the accuracy of the instrument's measurements using NIST SRMs. Generally, fuel contracts will explicitly state that in the event of a dispute over a fuel's sulfur content or the precision of an instrument that ASTM methods and NIST SRMs will be used to referee the dispute settlement.

Regulatory agencies use SRMs to support their quality control programs, which in turn play an important role in regulatory enforcement. To reduce the possibility of being out of compliance with environmental regulations, regulators and industry prefer to use the same standards and methods.

Regulators use SRMs to verify the calibration of their laboratory instruments with NIST SRMs. Like industry, regulators use NIST-traceable CRMs, which they may have purchased or prepared in-house, to calibrate equipment. The more expensive NIST SRMs are used at regular intervals to ensure the equipment is functioning properly.

NIST's SRM program supports the reproducibility and accuracy of the ASTM methods used to determine compliance by providing an authoritative primary standard. If SRMs were not available, greater uncertainty might occur regarding whether a plant was in compliance. Disagreements between a company and the regulatory agency regarding whether a plant was in compliance might result should a primary standard not be available.

C.3.2 SRM Customers

Table C-21 classifies the customers of the NIST SRMs under study for the past 9 years and shows the number of units purchased by each class of customers. From 1982 to early 1999, 2,954 different organizations purchased 45,673 units of sulfur fossil fuel SRMs.

Each level of the supply chain shown in Figure C-1 is represented among NIST's customers. As one would expect, among the largest group of customers are members of the sulfur measurement industry and members of the fuel extraction and processing industries. Public utilities are also important customers.

NIST SRMs are also purchased by users not specifically shown in Figure C-1. These companies include other U.S. industrial customers, such as cement and stone manufacturers, chemicals manufacturers, paper and allied products companies, and waste management companies. These companies could be using NIST SRMs to support sulfur measurements required for compliance with environmental regulations on industrial boilers. U.S. federal, state, and local governments also purchase NIST SRMs for environmental compliance purposes, and a number of foreign companies, universities, laboratories, and governments also purchase NIST SRMs for sulfur in fossil fuels.

Table C-21. Customers of NIST SRMs for Sulfur in Fossil Fuels Since 1982

Customers of NIST fossil fuel SRMs include members of each level of the supply chain, as well as a substantial number of government and private users from other countries.

Industry	Number of Customers	Number of Units Purchased
Measurement Industry		
Instrument Manufacturers	92	2,300
Reference Material Manufacturers	8	109
Laboratories, Consultants, and Universities	776	12,838
Fossil Fuel Extraction, Processing, and Transportation		
Fossil Fuel Extraction and Processing	455	12,191
Fuel Transportation and Export	95	903
Fossil Fuel Combustion		
Utilities and Utility Services	152	5,648
Steel Industry	33	301
Other U.S. Industrial Customers	358	3,501
Other SRM Users		
U.S. Federal, State, and Local Governments	212	1,265
Foreign Governments	77	542
Foreign Laboratories, Consultants, and Universities	233	1,312
Foreign Manufacturers	407	4,481
Unclassified	56	282
Total	2,954	45,673

Source: SRM purchase data provided by NIST's SRM program.

Table C-22 shows the number of customers by SRM and the total number of units purchased by SRM and customer type. The number of units of NIST SRMs purchased is lower for industry segments that are farther down the supply chain. This suggests that, while sulfur measurements at the top of the supply chain are often supported by NIST SRMs, downstream elements of the supply chain rely more heavily on secondary reference materials, which may, in turn, be supported by NIST SRMs.

Table C-22. SRM Purchases by SRM, 1982 to Early 1999

Industries farther down the supply chain use fewer NIST SRMs.

SRM	Description	First Certification Date	Number of Batches[a]	Number of Customers	Number of Purchases by Sector: Measurement Industry	Fuel Extraction, Processing, and Transportation	Fuel Combustion	Other SRM Users	Unclassified	Total
1616	Sulfur in Kerosene	2/19/88	2	442	442	658	102	212	2	1,416
1617	Sulfur in Kerosene	2/19/88	2	423	471	620	74	171	0	1,336
1619	Sulfur in Residual Fuel Oil, 0.7%	12/22/81	3	647	1,230	898	509	574	14	3,225
1620	Sulfur in Residual Fuel Oil, 4%	12/1/79	2	597	833	518	222	391	11	1,975
1621	Sulfur in Residual Fuel Oil, 1%	12/11/67	4	847	1,242	1,044	500	622	15	3,423
1622	Sulfur in Residual Fuel Oil, 2%	12/11/67	4	825	1,209	1,080	412	598	14	3,313
1623	Sulfur in Residual Fuel Oil, 0.3%	4/7/71	3	652	742	620	299	354	10	2,075
1624	Sulfur in Distillate Fuel Oil, 0.4%	4/7/71	3	643	496	786	247	396	10	1,935
1632	Trace Elements in Coal (Bituminous)	3/7/75	2	561	765	308	654	698	6	2,431
1633	Trace Elements in Coal Fly Ash	3/7/75	2	1,033	794	152	364	1,484	33	2,827
1635	Trace Elements in Coal (Subbituminous)	10/24/95	1	120	47	16	70	100	2	235
1819	Sulfur in Lubricating Base Oil	7/17/85	2	193	87	97	80	90	3	357
2294	Reformulated Fuels (nom. 11% MTBE, 35 mg/kg sulfur)	3/10/98	1	6	3	17	0	0	0	20
2295	Reformulated Fuels (nom. 15% MTBE, 300 mg/kg sulfur)	3/10/98	1	3	1	6	0	0	0	7

(continued)

Table C-22. SRM Purchases by SRM, 1982 to Early 1999 (continued)

					Number of Purchases by Sector					
SRM	Description	First Certification Date	Number of Batches[a]	Number of Customers	Measurement Industry	Fuel Extraction, Processing, and Transportation	Fuel Combustion	Other SRM Users	Unclassified	Total
2296	Reformulated Fuels (nom. 13% ETBE, 35 mg/kg sulfur)	3/10/98	1	2	1	1	0	0	0	2
2297	Reformulated Fuels (nom. 10% Ethanol, 300 mg/kg sulfur)	3/10/98	1	2	1	1	0	0	0	2
2682	Sulfur in Coal, 0.5%	12/14/82	2	473	702	864	818	286	6	2,676
2683	Sulfur in Coal, 2%	12/14/82	3	508	1,370	1,215	1,637	223	12	4,457
2684	Sulfur in Coal, 3%	12/14/82	2	427	1,663	1,170	1,410	182	122	4,547
2685	Sulfur in Coal, 5%	12/14/82	2	397	914	606	838	167	16	2,541
2690	Trace Elements in Coal Fly Ash	12/20/93	1	183	109	21	59	203	2	394
2691	Trace Elements in Coal Fly Ash	12/20/93	1	212	121	71	122	209	1	524
2692	Sulfur in Coal, 1%	11/15/88	2	288	1,059	478	679	281	0	2,497
2717	Sulfur in Residual Fuel Oil	10/25/90	1	299	378	346	107	185	2	1,018
2724	Sulfur in Distillate Fuel Oil, 0.04%	8/17/92	2	391	560	1,440	229	171	1	2,401
2775	Foundry Coke	5/12/99	1	14	6	7	17	3	0	33
2776	Furnace Coke	3/19/98	1	4	1	4	1	0	0	6
Totals			52	10,192	15,247	13,044	9,450	7,600	282	45,673

[a] Number of batches that were sold between 1982 and early 1999.

Source: Based on data provided by NIST's SRM program.