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MODULES FOR ESTIMATING SOLID WASTE FROM FOSSIL-FUEL TECHNOLOGIES

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ABSTRACT

Solid waste has become a subject of increasing concern to energy industries for several reasons. Increasingly stringent air and water pollution regulations result in a larger fraction of residuals in the form of solid wastes. Control technologies, particularly flue gas desulfurization, can multiply the amount of waste. With the renewed emphasis on coal utilization and the likelihood of oil shale development, increased amounts of solid waste will be produced.

In the past, solid waste residuals used for environmental assessment have tended only to include total quantities generated. To look at environmental impacts, however, data on the composition of the solid wastes are required.

Computer modules for calculating the quantities and composition of solid waste from major fossil fuel technologies were therefore developed and are described in this report. Six modules have been produced covering physical coal cleaning, conventional coal combustion with flue gas desulfurization, atmospheric fluidized-bed combustion, coal gasification using the Lurgi process, coal liquefaction using the SRC-II process, and oil shale retorting.

Total quantities of each solid waste stream are computed together with the major components and a number of trace elements and radionuclides.

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TABLE OF CONTENTS

Abstract iii

Acknowledgment iv

Introduction 1

1. Solid Waste Module for Physical Coal Cleaning 4
   References 31
   Appendix 1A 32
   Appendix 1B 34
   Appendix 1C 41
   Appendix 1D 44

2. Solid Waste Module for Coal Combustion in a Conventional Boiler 54
   References 76
   Appendix 2A 78
   Appendix 2B 94
   Appendix 2C 103
   Appendix 2D 107

3. Solid Waste Module for Atmospheric Fluidized Bed Combustion 118
   References 131
   Appendix 3A 132
   Appendix 3B 139
   Appendix 3C 142

4. Solid Waste Module for Lurgi Process Coal Gasification 150
   References 164
   Appendix 4A 165
   Appendix 4B 171
   Appendix 4C 178
   Appendix 4D 180

5. Solid Waste Module for the SRC-II Process Coal Liquefaction 186
   References 198
   Appendix 5A 199
   Appendix 5B 202
   Appendix 5C 208
   Appendix 5D 210

6. Solid Waste Module for Oil Shale Retorting 216
   References 229
   Appendix 6A 230
   Appendix 6B 232
   Appendix 6C 234
   Appendix 6D 236

7. Radionuclides 243
   References 249

TABLES

1.1 Typical Size Distribution of Coals 19

1.2 Elements 22

1.3 Coefficients Used to Determine Percentage Recovery of Trace Elements 28

1B.1 Example of Calculation of Fractionation Factor Using Results for Nickel 34

1B.2 Trace Metal Coal Cleaning Data 36

1B.3 Key to Trace Metal Factors 38

1B.4 Trace Element Recovery as a Function of Ash or Pyritic Sulfur Recovery 40

1D.1 Input Characteristics of Coal 44

2.1 Elements 61

2.2 Boiler Coefficients for Fraction of the Incoming Element which Goes Up the Stack 63

2.3 Coefficients for Calculation of Air Emissions 66

2.4 Coefficients to Calculate the Function of a Trace Element Passing Through a Precipitator 67

2.5 Coefficients to Calculate FGD Sludge and Its Major Components for Wet Scrubbing Systems 69

2.6 Fraction of Trace Elements in Lime and Limestone 70

2.7 Coefficients to Calculate FGD Waste and Its Major Components for a Dry Sorbent Injection System 74

2A.1 Fraction of Elements Entering with Coal Discharged in Bottom Ash or Sluice Ash for Sampled Stations 79

2A.2 Fraction of Elements Entering with Coal Discharged in Economizer Ash Plus Scrubber Slurry or Cyclone Ash or Precipitator Ash for Sampled Stations 79

2A.3 Fraction of Elements Entering with Coal Discharged in Flue Gas for Sampled Stations 80

2A.4 Calculation of Average Percentage of Trace Elements which Remain in the Bottom Ash in a Pulverized Utility Boiler 80

2A.5 Distribution of Trace Elements for a Cyclone Boiler Normalized to Give a Mass Balance of 100%, Reference 5 (1972) 82

2A.6 Distribution of Trace Elements for a Cyclone Boiler Normalized to Give a Mass Balance of 100%, Reference 5 (1973) 82

TABLES (Cont.)

2A.7 Calculation of Average Percentage of Trace Elements which Remain in the Bottom Ash in a Cyclone Utility Boiler 83

2A.8 Distribution of Trace Elements, Pulverized Boiler, Station I, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas 84

2A.9 Distribution of Trace Elements, Pulverized Boiler, Station II, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas 84

2A.10 Distribution of Trace Elements, Pulverized Boiler, Station III, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas 85

2A.11 Distribution of Trace Elements, Reference 5 (1972), Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas 85

2A.12 Distribution of Trace Elements, Reference 5 (1973), Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas 86

2A.13 Percentage Pass-Through of Trace Elements for Precipitators of Varying Efficiency 88

2A.14 Enrichment of Trace Elements upon Passing through Precipitator 88

2A.15 Ratios of Pass-Through of Trace Elements at Four Power Plants 89

2A.16 Theoretical Proportions of Trace Metal Pass-Through for Given Functions of Fly Ash Pass-Through 89

2A.17 Relation of Particulate Pass-Through to Enriched Trace Element Pass-Through for Enriched Trace Elements 92

2A.18 Percentage Pass-Through of Trace Elements as Compared to the Pass-Through of Fly Ash for a Scrubber........

2B.1 Default Values for Calculation of FGD Solid Waste 93

2B.2 Molecular Weights of Compounds Used in FGD Systems 95

2D.1 Input Characteristics of Coal 95

3.1 Elements 107

3.2 Composition of Spent Sorbent Material 128

3.3 Total Solid Waste Distribution 129

3.4 Coefficients for the Distribution of Elements Between Output Streams 130

TABLES (Cont.)

3C.1 Input Coal Characteristics 143

3C.2 Input Limestone Characteristics 143

4.1 Elements 161

4.2 Fractions (Coefficients) of Array Elements Going to Solid Waste Streams 162

4.3 Estimation of Water and Total Solid Waste 163

4A.1 Coal Characteristics, Total Waste Streams, Water Content 166

4A.2 Carbon Distribution 167

4A.3 Sulfur Distribution 169

4A.4 Ash Distribution 170

4B.1 Coal Content of Trace Elements (ppm) 171

4B.2 Fraction of Input Trace Elements in Bottom Ash 173

4B.3 Fraction of Input Trace Elements in Oil 174

4B.4 Fraction of Input Trace Elements in Tar 175

4B.5 Fraction of Input Trace Elements in Gas Liquor 176

4D.1 Input Characteristics of Coal 180

5.1 Summary of Solid Wastes Control Technology Applicability to SRC Systems 191

5.2 Elements 195

5.3 Fractions (Coefficients) of Array Elements Going to Solid Waste Streams 196

5.4 Determination of Total Output and Major Components 197

5B.1 Trace Element Content of "Average U.S. Coal" 203

5B.2 Partitioning Factors and Proportion of Total Trace Elements Retained in Mineral Residue 205

5B.3 Trace Elements in Slag, Recovered Sulfur, and SRC Product 206

5D.1 Input Characteristics of Coal 210

6.1 Solid Waste Other than Spent Shale 222

6.2 Elements 226

6.3 Coefficients for Total Output and Major Components for TOSCO II 227

6.4 Coefficients for Total Output and Major Components for Paraho 227

TABLES (Cont.)

6.5 Fractional Split of Trace Elements between Spent Shale and Oil 228

6D.1 Input Characteristics of Oil Shale 236

7.1 Uranium Series Main Decay Chain (Minor Side Chains Excluded) 244

7.2 Actinium Series Main Decay Chain (Minor Side Chains Excluded) 245

7.3 Thorium Series Main Decay Chain (Minor Side Chains Excluded) 245

FIGURES

1.1 Level 1 Preparation 10

1.2 Level 2 Preparation 12

1.3 Level 3 Preparation 16

1.4 Overall Coal Cleaning Module Design 21

2.1 Overall Conventional Combustion Module Design 57

3.1 AFBC Conceptual Plant Design 120

3.2 Overall AFBC Module Design 125

4.1 Schematic Flow Diagram of a Coal Gasification Plant 153

5.1 Flow Diagram of a SRC-II Operation 188

5.2 Sources of Solid Wastes in SRC Systems 192

6.1 Paraho Process 219

6.2 TOSCO II Process 220

6.3 Overall Oil Shale Module Design 224

INTRODUCTION

The Environmental Impacts Division, Office of Environmental Assessments, U.S. Department of Energy, has given Brookhaven National Laboratory the overall responsibility for developing a capability for assessing energy production solid waste problems and impacts. As part of this effort, the Biomedical and Environmental Assessment Division has developed six computer modules, in the form of FORTRAN subroutines, which can be used to estimate total solid waste and the composition of that waste for six fossil fuel technologies (coal combustion in a conventional boiler, coal beneficiation, coal gasification, SRC-II process coal liquefaction, oil shale recovery, and atmospheric fluidized-bed combustion). These modules were written so that they could be used as individual programs for estimating solid waste in a single situation, or, could be included in a larger overall system of environmental assessment. In this report, each module is described and documented in detail. Computer codes and technical explanations of the calculations are appended to each section.

At present, in the Strategic Environmental Assessment System (SEAS), only the quantities of solid waste are calculated; no assessment is made of the composition of the waste either in terms of its major constituents or its trace element content. The composition of the waste is needed in order to determine disposal methods and potential environmental impacts. No estimation of the environmental impact of solid waste disposal is at present given in SEAS.

The Regional Studies Group at BNL is preparing an overall model to evaluate the impact of solid waste disposal from energy production. An important part of the model is the computation of the quantity and composition of the solid waste produced from different energy production processes. This will be achieved by a series of modules, each representing a specific technological process and producing information about the waste (amount and chemical composition) as a function of fuel input and, as needed, other information supplied exogenously to satisfy the requirements of the individual modules.

In an overall model framework such as these, the modules can be linked in series (e.g., coal beneficiation, coal combustion). Regulatory considerations are included in the main program; modules contain variables to simulate the technological response to changes in regulation. In an overall evaluation framework, regulatory and locational considerations can be used in conjunction with the coal input characteristics to specify emissions limits options in the technology modules. These considerations will also dictate the sequence of decisions which determines the management of the solid wastes (e.g., the regionally available method, need for full containment, etc.).

Since the modules will be used primarily in larger environmental assessment models such as those mentioned above, the individual modules used to compute the solid waste produced need to be mathematically simple so they may be called many times during a run of the overall program. Also, since at present the modules are data limited, they were written in such a way as to allow easy updating of coefficients when new data become available.

The modules are generally based on a mass balance approach and consist of one or more matrices of coefficients which, when multiplied by a vector of input fuel characteristics, results in a matrix describing the characteristics of one or more products and waste streams. The modules, however, remain a flexible means of coping with changes in air pollution control requirements, and in cases where there are various possible technologies (e.g., flue gas desulfurization (FGD) systems in conventional boiler coal combustion), they allow for a number of possible choices.

In many cases there is a linear relationship between the fuel characteristics and the residual characteristics for a specific technology. In those cases where this may not be the case, nonlinear functions are incorporated into the module.

Composition of the Solid Waste

The modules take run-of-mine (ROM) fossil fuel characteristics and compute their fate during a combustion or conversion process. A choice had to be made as to which constituents should be considered.

For the major components, mass balances are calculated for sulfur, ash, and carbon. For the trace constituents, the trace elements listed by the EPA as toxic under the Clean Water Act were used (Federal Register, Vol. 44, No. 191, Monday, October 1, 1979). In addition, iron, magnesium, and manganese were added.

The full list of trace elements considered is given below:

Antimony
Arsenic
Beryllium
Cadmium
Chromium
Copper
Magnesium
Manganese
Mercury
Nickel
Selenium
Silver

Iron
Lead
Thallium
Zinc

Radionuclides are also important in describing solid waste, and the following were included in the modules:

Uranium
Radium
Thorium
Lead-210

The reasons for inclusion or exclusion of certain radionuclides are given in Section 7.

While the main purpose of the modules is to describe solid waste characteristics, the composition of product streams and air residuals is also included in some of the modules.

Note: The results obtained by using the described computer modules should be considered only as good as the data used in determining the coefficients. As will be seen, data are often scarce and sometimes nonexistent. Some of the data used are suspect. Therefore, results should be regarded as only a general guideline to the actual composition of the solid waste from the fossil fuel technologies considered. In the future, it is hoped that more and better data will be collected so that the present coefficients can be updated to improve the accuracy of estimation.

1 SOLID WASTE MODULE FOR PHYSICAL COAL CLEANING

1.1 Introduction

Physical coal preparation consists of the mechanical cleaning and sorting of particles of coal and its impurities.

1.1.1 Why Steam Coals Are Beneficiated

Historically, only coals intended for metallurgical purposes were beneficiated to reduce their ash content. Steam coals were washed only when the raw coal, ROM, contained unacceptably high proportions of ash-forming minerals. Whereas power plants can often cope with ash contents of 20 percent or higher, some ROM coals contain up to 40 percent ash, and occasionally even more. When lower sulfur oxide emissions were mandated by the 1970 Clean Air Act, coal beneficiation to reduce sulfur content gathered momentum. In light of the latest environmental developments, it is reasonable to expect that steam coal beneficiation will become increasingly important as a major BACT (Best Available Control Technology) and will be used with flue gas cleanup systems to meet increasingly strict sulfur controls. In other cases, coal beneficiation willpay for itself because the enrichment of the shipped product reduces freight costs.

1.1.2 Coal Beneficiation Principles

With few exceptions, all washed coals are processed in water or water-based media, using gravity methods which rely on the differences in specific gravity between the coal and minerals mixed therewith. Only extraneous impurities are separable from the coal proper, although the efficiency of such separation varies with the coal's characteristics.

A jig, the most popular coal-washing device, uses differential settling or induced stratification to separate the lighter coal from the heavier ash-forming minerals. Next in popularity is the heavy-media process. With this method, the coal is floated in a water-based medium of controlled specific gravity and the heavier minerals are permitted to sink and be removed as rejects. The concentrating table separates coal from rejects by stratification induced by vibration. Cyclones, either water-only or heavy-media types, supplement gravity by centrifugal force to make sharper separations than static vessels. Froth flotation, which is used with coal particles smaller than 28 mesh (1/2 millimeter), uses chemical reagents to form air bubbles which selectively attach themselves to the coal while permitting the ash to settle to the bottom.

Because any coal particle contains both coal and ash, its specific gravity will depend on the relative percentages of each. Pure coal has a specific gravity slightly less than 1.3, whereas a dirty coal containing approximately 60 % ash has a specific gravity of about 1.8. Most clean coals are produced with specific gravities between 1.4 and 1.6 and contain upward of 5 % ash. The smaller the particle's size, the better the chance of separating the coal from its ash but also the higher the processing costs. As pyritic sulfur is associated with ash and has an even greater specific gravity, sulfur reduction methods are essentially the same as those used for ash reduction and are subject to the same limitations.

1.1.3 Levels of Coal Preparation

The extent of the work done on raw coal is determined by marketing considerations and by the results of float-sink tests called coal washability analyses. There are substantial differences in the degree to which any coal can be improved by beneficiation. In the past it was primarily the ash content of a coal which had to be limited, and the smallest amount of preparation to meet that criterion was used. Since the advent of the Clean Air Act, more steam coal specifications call for quality products achievable only through beneficiation. Costs associated with coal beneficiation reflect the level of preparation practiced. Obviously, crushing only to control top size is far less costly than beneficiation to reduce ash and sulfur content. Coal preparation can be classified according to the sizes of coal particles processed. The smaller the particles, the more rigorous the level of beneficiation, the more complex and costly the process, and the better the product.

Coal preparation processes are usually designed and operated for site specific applications. Plants can be loosely grouped as jig plants, table plants, and heavy media plants. As plants frequently use at least two, if not all three, of these methods simultaneously and at times flotation, this classification has limited usefulness. Professor H. Lovell[1] of Pennsylvania State University defines four levels of preparation. At one end, level 1 employs no preparation at all, while at the other end, level 4 calls for multistage beneficiation. Gibbs and Hill Inc. in a report prepared for EPRI[2] proposes that at least six levels are required to represent the most basic differences:

Level 0: Absence of preparation indicates that the coal is shipped as mined.

Level 1: Breaking for top size control only, with limited, if any, removal of coarse refuse and trash.

Level 2: Coarse beneficiation through washing of >3/8-in. material only: 3/8-in. x 0 fraction remains dry and is recombined with the clean coal prior to shipment.

Level 3: Deliberate beneficiation through washing of all >28 mesh material; 28-mesh x 0 material, depending on its quality, is either dewatered and shipped with clean coal or discarded with the refuse.

Level 4: Elaborate beneficiation through washing of all size fractions, including 28 mesh x 0. Thermal drying of 1/4-in. x 0 sizes is generally required to limit moisture content.

Level 5: Full beneficiation implies the most rigorous coal beneficiation.

At present, levels 1 and 2 are used to clean steam coal and levels 4 and 5 are used for metallurgical coal.

Level 3 improves the quality of the coal over that of level 2 by cleaning the 1/4-in. x 28-mesh size which normally contains large amounts of sulfur.

The present module will allow the calculation of solid waste for coal cleaned at levels 1 to 3. If in the future it is felt the utilities may use coal that has been beneficiated to metallurgical standards, levels 4 and 5 could be added. However, the module will become more complicated and data restrictive as the level of cleaning increases, particularly since levels 4 and 5 would require thermal drying of the coals.

Each of the three levels to be employed in the module is discussed in greater detail below.

Preparation Level 1 - Breaking Only

Block Diagram: Figure 1.1.

Scope: Top size control through crushing only prior to storage and/or shipment. In this context, level 1 preparation does not include physical coal preparation processes such as crushing, grinding, classifying, slurrying and dewatering, compacting, and pelletizing.

Purpose and Benefits: Except for the relatively few mines able to ship ROM coal directly to the user, most mines must control the top size of the raw coal to facilitate handling and to suit customer requirements. Normally there is little improvement in coal quality as a result of crushing the coal prior to shipment, except possibly in northern West Virginia, and in parts of Ohio, Pennsylvania, and Illinois, where large formations of pyritic sulfur are sometimes encountered. Unless removed by a rotary breaker, these very hard lumps can damage crushers. Wood and timber can also be removed from the ROM feed by a rotary breaker.

Ash Reduction: Negligible.

Sulfur Reduction: Negligible.

Yield - Weight Basis: 98 to 100%.

Recovery - Btu Basis: 99 to 100%.

Major Circuits and Equipment Used: Size reduction is accomplished by means of crushers and/or rotary breakers. Scalping screens (coarse screens) are frequently used ahead of crushers and breakers either to remove large wood and timbers likely to plug the crushers or to bypass the crushers with coal particles already small enough. Breakers work

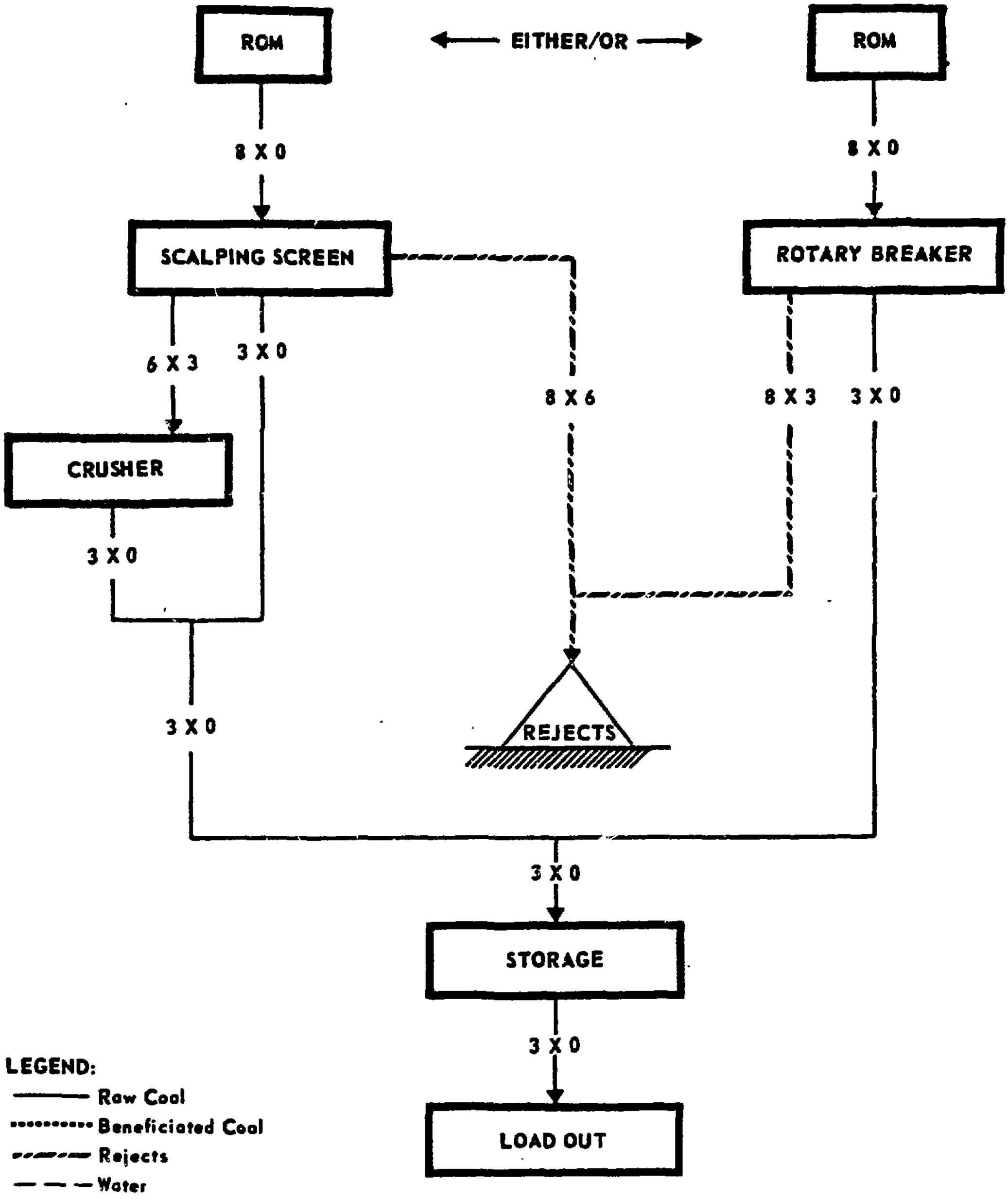

Figure 1.1. Level 1 preparation. (From Reference 2.)

when the coal is soft and the rock is hard because they size and recover all coal and reject large rock, wood, timber, and trash.

When the coal is hard or tough, single or double roll crushers are used, preceded by scalping screens. Where ROM coal is relatively clean and where wood and timbers are no problem, rotary breakers are sometimes sealed, preventing discharge of rejects. In this way they act like single roll crushers but their maintenance costs are lower.

Strip-mined subbituminous coals and lignites are reduced in size by means of roll crushers when trash is not a problem. Breakers are used when seams are contaminated with rocks or petrified wood.

Rejects Processing and Disposal: Disposal is usually by truck to the mine refuse area where it is layered and compacted by a bulldozer at the head of the valley. This material is usually dry and coarse. Thus, drainage and seepage are not a problem nor is spontaneous combustion.

Preparation Level 2 - Coarse Beneficiation

Block Diagram: Figure 1.2.

Scope: After level 1 preparation, remove the 3/8-in. x 0 particles by dry screening. Wet beneficiate only the >3/8-in. coal, then dewater by mechanical means and ship after recombining with the unprocessed 3/8-in. x 0 raw coal fines. Where raw coals do not contain excess surface moisture (because of dust control sprays at mine face) likely to plug the screen openings, dry screening at 1/4 in. is preferred.

Purpose and Benefits: Coarse beneficiation removes the coarse impurities (above 3/8 in.) often found within coal seams, such as partings and the

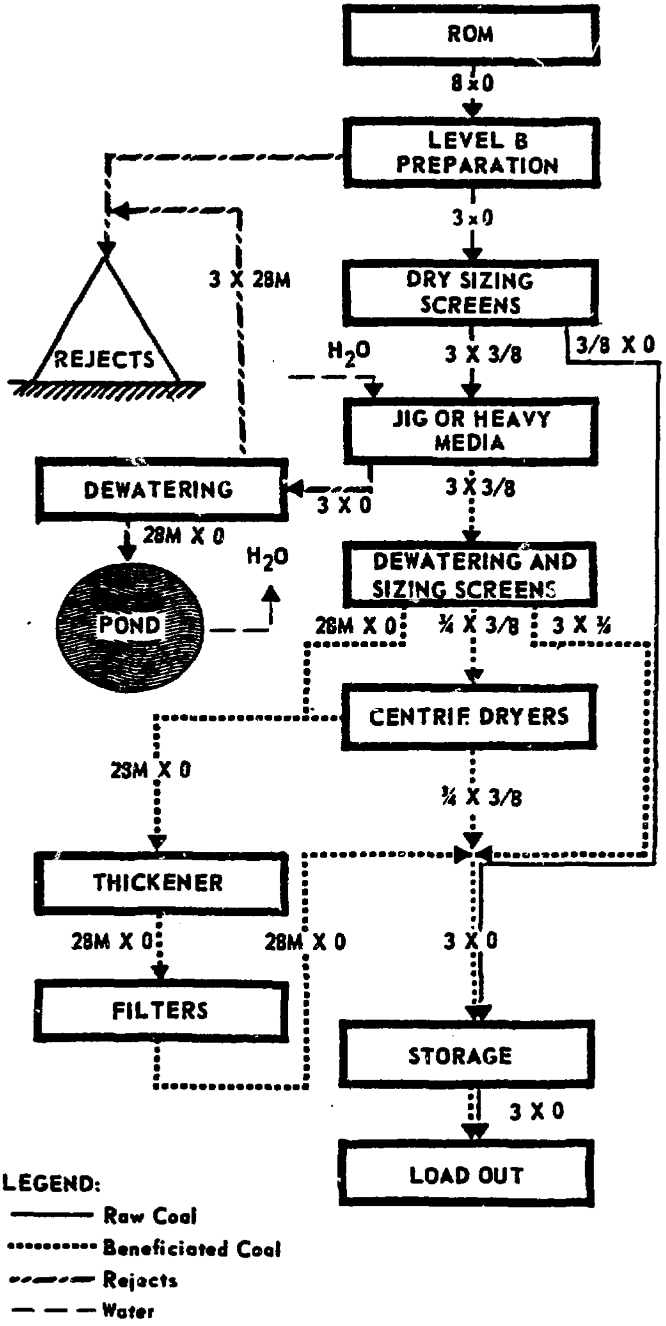

Figure 1.2. Level 2 preparation. (From Reference 2.)

extraneous material (roof and bottom) extracted with the coal as a result of big production mining procedures. The 3/8-in. x 0 raw coal split remains as mined and rejoins the clean coal stream prior to shipment. Although coarse beneficiation can remove substantial quantities of extraneous matter which would otherwise show up in ash analysis of the coals, substantial sulfur reduction should not be expected as sulfur particles are generally not associated with the coarse rejects. Coarse beneficiation of steam coals is practiced on coals from Appalachia and Alabama which have excellent washability characteristics and where the ash content of the coal fines is not excessive. 28-mesh x 0 coal from an Appalachian seam, for example, contains less than 22%ash, whereas the same split from an Illinois seam might run up to 40%ash.

Ash Reduction: Fair to good; can compensate for poor quality control at the mine face.

Sulfur Reduction: Minor as the coarse rejects rarely contain much sulfur.

Yield - Weight Basis: 75 to 85%.

Recovery - Btu Basis: 90 to 95%; Btu recovery is good because few of the coarse rejects, except bone coal, contain many Btu.

Major Circuits and Equipment Used: ROM coal is first reduced in a level 1 circuit to <3 in. (3 in. is used as an example). Further reductions to 3/4 in. or less may be more desirable, but each coal must be evaluated individually. Crushed coal is then dry screened at 3/8 in. to remove the fines which bypass the beneficiation circuits and eventually rejoin the washed coal.

The >3/8 in. fraction is beneficiated in jigs or heavy media vessels at a relatively high specific gravity (1.50 to 1.55) to reduce the amount of coal included with the rejects (refuse). The clean coal fraction is then passed over dewatering and sizing screens. The coarsest fraction (>3/4 in.) contains relatively little surface moisture and can be shipped without further treatment. The 3/4-in. x 3/8-in. split must be dewatered in mechanical dryers, while the limited amount of 28-mesh x 0 washed from the clean coal discharges either to a thickener and filters or to a settling pond. The clean coal, combining the 3/8-in. x 0 dry screened fraction, the >3/8-in. washed fraction, and the 28-mesh x 0 filter product may contain slightly more surface moisture than the ROM coal, but not enough to cause transportation or utilization problems.

Rejects Processing and Disposal: The dry refuse from level 2 can be discarded as discussed earlier. The rejects from jigs or heavy-media vessels consist of wet, >3/8-in. refuse and a <28-mesh slurry. The slurry is either discharged to a settling pond or reports to a thickener for water clarification and recovery. If a thickener is used, the underflow (water and suspended solids) might have to be ponded. Because of regulatory restrictions on the use of ponds and impoundments, their use is decreasing in favor of centrifuging and filtering. The >3/8 in. rejects may contain from 6 to 12% surface moisture, depending on top size. This refuse, which can represent 15 to 40% of the raw coal, must be transported to, and confined within, a suitable disposal area constructed, operated, and maintained in accordance with applicable regulations.

Preparation Level 3 - Deliberate Beneficiation

Block Diagram: Figure 1.3.

Scope: After level 1 preparation, the 3/8-in. x 0 particles from the 3-in. x 0 feed are separated by wet screening, followed by a second separation at 28 mesh. The >3/8 in. coal is washed as in level 2. The 3/8-in. x 28-mesh is beneficiated on concentrating tables or in heavy-media cyclones, followed by dewatering screens and centrifugal driers. The 28-mesh x 0 split is combined with the same size product from other circuits and, although not beneficiated, is thickened and filtered prior to rejoining the clean coal stream for shipment.

Purpose and Benefits: Level 3 coal preparation further improves quality by beneficiating the 3/8-in. x 28-mesh size which normally contains large amounts of ash and sulfur. As this fraction may roughly constitute one third of the plant feed, the quality of the clean coal will favorably reflect the work done on the 3/8-in. x 28-mesh split.

Ash Reduction: Good to excellent.

Sulfur Reduction: Fair to good.

Yield - Weight Basis: 60 to 80%.

Recovery - Btu Basis: 80 to 90%; as the finer coal sizes are more difficult to beneficiate, the percentage recovery decreases in comparison with level 2.

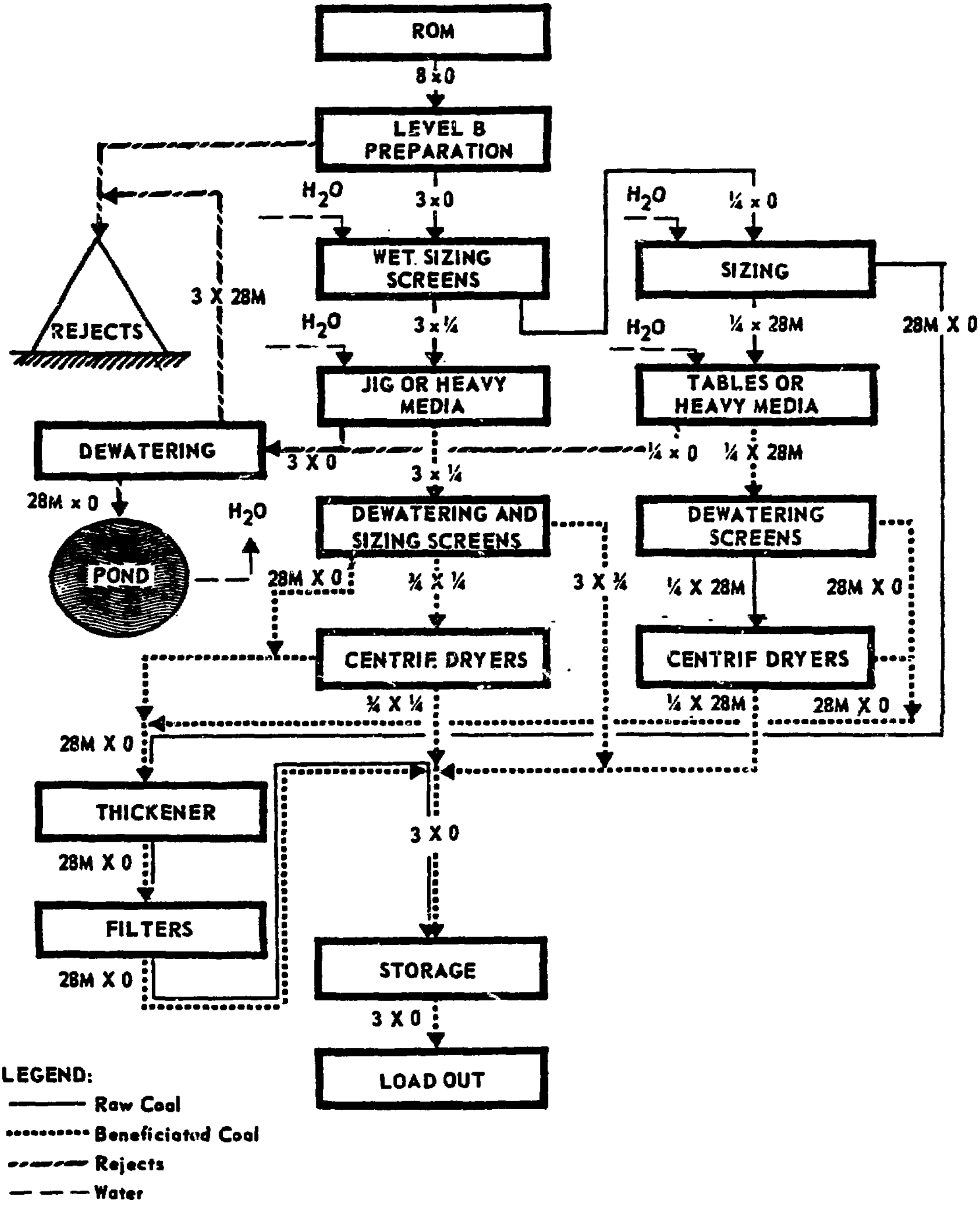

Figure 1.3 Level 3 preparation. (From Reference 2.)

Major Circuits and Equipment Used: The circuits are those required for a level 2 plant, plus those for beneficiating the 3/8-in. x 28-mesh coal. Concentrating tables or heavy-media cyclones are suitable, followed by mechanical dewatering. Thickeners and filters, preceded by classifying cyclones, are used when the <28-mesh percentage is high and are used both for the clean coal and the rejects when ponding is unavailable.

Rejects Processing and Disposal: Problems encountered with rejects from level 2 plants are accentuated in level 3 plants which must dispose of even greater amounts of wetted fines, particularly the 28-mesh x 0 fraction. When the <28 mesh slurry contains clay (southern Illinois strip mines, for example), it must be pumped to impoundment areas, as filters cannot efficiently handle clays. Legal restrictions on such impoundments sometimes effectively prohibit their use or at least increase their construction costs. Dams costing several million dollars are not unheard of. In flat terrain, the problem may be practically insurmountable because of the large quantities involved. The 3/8-in. x 28-mesh refuse contains 17 to 22% moisture, depending on dewatering methods employed and the 28-mesh x 0 fraction, after filtering, will contain 15 to 25% moisture. The 3/8-in. x 0 rejects pose handling problems, not only during freezing temperatures but also at other times because such refuse is difficult to convey or truck without spills or leaks. Disposal is complicated by detailed regulations including prohibition on effluent.

1.1.4 Modeling Problems

Coal preparation is very site specific; every plant is built differently because of the large variation in the washability of different coals. This causes a number of problems when trying to build a model which will have to deal with cleaning in a general manner.

A brief description of the major problems encountered and the methods used to overcome them is given below.

Pyritic Sulfur and Ash Removal. Given a specified level of cleaning, the amount of pyritic sulfur removed will vary with each coal sample (variations may be found even within the same coal bed). To a lesser degree, this is also true of ash removal.

The U.S. Bureau of Mines[3] has performed washability studies on 455 samples of coal. These results were used to determine if it was possible to correlate pyritic sulfur with ash removal, Btu loss, and overall material loss. Details are given in Appendix 1A.

Trace Metal Removal. As with pyritic sulfur, the removal of trace metals will also vary, depending on the coal type used.

Data from a number of float sink tests which looked at the fate of trace metals were used to determine if a function could be found which related trace metal removal with pyritic sulfur or ash removal. Details are given in Appendix 1B.

Size Distribution of the Coal. As can be seen from the block diagrams, the amount of coal cleaned at each level and hence the amount of solid waste will depend on the size distribution of the coal after crushing.

Although the size distribution is not a haphazard event, the equations used to calculate the distribution require constants which vary for each coal type and depend on such properties as the friability of the coal. Distributions cannot be calculated in the module and therefore a number of typical size distributions were examined and the average taken (Table 1.1).

Table 1.1
Typical Size Distribution of Coals

	>3/8 in.	3/8 in.-28 mesh	<28 mesh
Reference 4			
Nat. ave. steam cleaning	72.0	28.0	
Nat. ave. metallurgical cleaning	53.2	40.0	6.8
Central region ave.	56.0	44.0	
Northern Appalacian region	72.0	28.0	
Reference 5			
Freeport, Pennsylvania	77.0	19.0	4.0
Crushed Freeport, Pennsylvania	60.0	34.0	6.0
Roslyn bed, Washington	70.0		
Alabama	60.0	34.0	6.0
Reference 2			
Alabama	70.0	23.0	7.0
Average	65.6	27.8	6.0

The module assumes the following split:

>3/8 in.	66%
3/8 in - 28 mesh	28%
<28 mesh	6%

1.2 Coal Cleaning Module Description

1.2.1 General Description

The module computes the solid waste residuals and the clean coal characteristics which result from physical coal cleaning at three levels of intensity.

The input to the module is the quantity of coal and its composition in terms of sulfur (pyritic and organic), ash, trace elements, and Btu content. The module employs a mass balance approach to compute the distribution of the sulfur, ash, and trace elements between the clean coal and the solid waste refuse. Figure 1.4 gives an overall view of the module.

For levels 2 and 3, the equations used to compute the solid waste produced are valid only when the input ash content of the coal exceeds 6.25%. This is thought to be reasonable since it is unlikely that it would be economical to try to clean a coal with a lower ash content. Low ash coals normally have low sulfur contents.

Since thermal drying is not being considered, the only air emissions are fugitive dusts, which are difficult to quantify. No air emission estimates are therefore included.

The module is called as a subroutine with the following arguments:

Input vector of coal characteristics.

Output vector of clean coal composition.

Output vector of solid waste composition.

Input quantity of coal/output quantity of coal.

Level of coal preparation. Input integer number from 1 to 3.

To facilitate computation, the first three arguments are vectors which contain the same number of elements. The elements are shown in Table 1.2. Since these vectors are constructed to be conformable to any of the solid waste modules which have been produced, there are presently some empty elements (48 to 50, not shown in Table 1.2) and some elements which are not applicable to this module and are disregarded (set to 0) in the output vectors and omitted in the output printout.

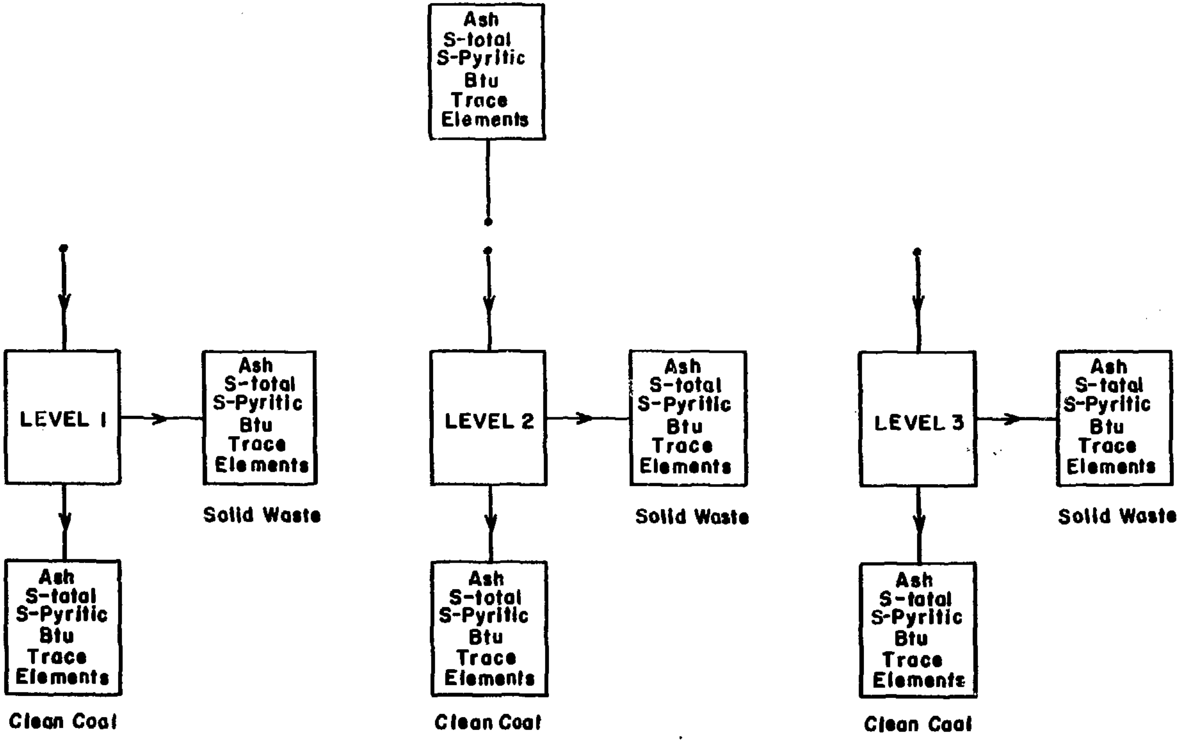

Figure 1.4. Overall coal cleaning module design.

Table 1.2
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

Data are, at present, only generally available for the input quantities of uranium and thorium. However, the masses of radium-226 and lead-210 can be calculated from the mass of uranium-238 and the mass of radium-228 from thorium-232. The equations and assumptions used in the calculation are given in Section 7.

It is assumed for each level of cleaning that the percentage carbon reduction is equivalent to the percentage Btu loss.

For each level of cleaning, there will be an output vector of clean coal characteristics and of solid waste quantity and composition. Also given is the output quantity of clean coal. The total Btu's in the clean coal are given in the output clean coal vector and therefore the new Btu/lb can be calculated, if required, for further analysis.

1.2.2 Level 1 Cleaning

The module assumes a 99.5% Btu recovery and a 98% material recovery. These are average figures from References 2, 4, and 6.

The solid waste will therefore contain 0.5% of the input carbon. The fraction of the ash removed can then be calculated using the following equation:

$$\text{ASHREM} = (0.02 \times \text{COAL}) - (0.005 \times \text{CARBON})/(\text{COAL-CARBON}),$$

where

ASHREM is the fraction of incoming ash removed,

COAL is the total quantity of input coal,

CARBON is the input quantity of carbon.

With the exception of sulfur, the same removal fraction as ash is used for the other trace elements.

The pyritic sulfur is assumed to be reduced by the same amount as the ash, but the organic sulfur is removed at the same rate as the carbon. Organic sulfur is not given as a separate input element but is calculated as the difference between the total and pyritic sulfur.

There are two output vectors to describe the clean coal and solid waste composition. The total solid waste (element 25) is assumed to be a dry weight.

1.2.3 Level 2 Cleaning

The module assumes an overall Btu recovery of 93% (average value from references 2, 4, and 6). However, only the >3/8-in.fraction of the coal is being cleaned. This constitutes 66% of the input coal (see Section 1.4.4) and therefore the Btu recovery for the coal subject to cleaning is 89.4%.

Major Components. The major components of the solid waste are carbon, sulfur, and ash.

Physical cleaning removes only pyritic sulfur. However, since there is some carbon removal it is assumed that there will also be a small reduction in organic sulfur.

The major components of the waste are calculated using the following equations. Those for total waste and pyritic sulfur were derived from the results of the washability studies performed by the Bureau of Mines.[3] Details on how the equations were derived are given in Appendix 1A. These equations are applied to only 66% of the incoming coal.

Total Solid Waste (Dry Weight)

$$\text{COALR} = 0.719 \times \text{A} + 0.890 \times \text{BTUR} - 3.698$$

$$\text{TSW} = \text{QCOAL} \times (\text{COALR}/100),$$

where

COALR is the percentage material removal,

A is the ash content of input coal (%),

BTUR is the percentage Btu removal,

TSW is the total quantity of solid waste,

QCOAL is the input coal quantity.

Carbon Content of Solid Waste

$$CSW = QC \times (BTUR/100),$$

where

CSW is the quantity of carbon in the waste,

QC is the input quantity of carbon.

Hydrogen, Oxygen and Nitrogen Content of the Solid Waste. Although hydrogen, oxygen, and nitrogen are not considered as elements in the module, their presence in the coal affects the amount of ash in the solid waste. They are assumed to be present in the solid waste in the same proportion as the carbon removal.

$$OHNSW = (QCOAL - QC - QA - QS) \times (BTUR/100),$$

where

OHNSW is the total quantity of hydrogen, nitrogen, and oxygen in the solid waste,

QA is the input ash quantity,

QS is the input sulfur quantity.

Ash Content of Solid Waste

$$ASW = TSW - CSW - OHNSW,$$

where

ASW is the amount of ash in the solid waste.

Sulfur Content of Solid Waste

Organic Sulfur

$$OSSW = QOS \times (BTUR/100),$$

where

OSSW is the quantity of organic sulfur in the solid waste,

QOS is the quantity of organic sulfur in the input coal.

Pyritic Sulfur

$$PSR = 0.686AR + 3.578 \ln(PS) + 2.499\, BTUR$$
$$+127.286 \ln(100 - COALR) - 584.565,$$

$$PSSW = QPS \times (PSR/100),$$

where

PSR is the percentage removal of pyritic sulfur,

AR is the percentage removal of ash,

PS is the percentage of pyritic sulfur in the input coal,

PSSW is the quantity of pyritic sulfur in the solid waste,

QPS is the input quantity of pyritic sulfur.

Total Sulfur

$$SSW = OSSW + PSSW \text{ tons},$$

where

SSW is the total quantity of sulfur in the solid waste.

Trace Components. A number of workers have performed float-sink tests on coal samples to determine the fate of trace elements during washing.

H.J. Gluskoter and his colleagues have investigated the trace element content of coal for the Illinois State Geological Survey. In Reference 7, nine coal samples were crushed to 3/8-in. top size and the 3/8-in. x 28-mesh fraction was subjected to specific gravity separation. One set of samples had very poor mass balances and contained some spurious results; the data for one set were incomplete so the results from 7 samples were used in this analysis.

C.T. Ford of the Bituminous Coal Research Institute has recently been studying the effect of washing on the trace element content of coal. Unfortunately, the only results now available are from a symposium held in 1977[8], but a report is being compiled which will give more recent results. Reference 8 describes specific gravity separations performed on 8 samples using the 3/8-in. x 0 size.

These two sets of experiments examined a large number of trace elements. Two further reports were used but in these only a limited range of trace elements were measured. J.A. Cavallaro and colleagues[9] at the Bureau of Mines reported on the results for specific gravity separation of 14-mesh top size samples of 10 coals; in another report[10] they look at 4 samples again crushed to 14-mesh top size.

The results were used to calculate the fraction of each trace element that remained with the clean coal. The fractions were normalized to assume a 100% coal recovery level. Details of how the fractionation factors were calculated are given in Appendix 1B.

These figures were used to determine whether there was any correlation between the recovery of a particular trace element and the recovery of pyritic sulfur or ash. In many cases, equations could be found which gave the recovery of a trace element as a function of the ash or pyritic sulfur recovery. In some cases, no correlation was found and an average value is used.

Table 1.3 gives the coefficients used to determine the recovery of trace elements; details of how they were obtained are given in Appendix 1B. Again, these coefficients are applied to 66% of the coal.

Table 1.3
Coefficients Used To Determine Percentage Recovery of Trace Elements

Element	Coefficient (% Recovery)
Antimony	85.0
Arsenic	A
Beryllium	$4.641 \sqrt{A} + 49.713$
Cadmium	$\ln$ (Cd recovery) = $0.006S + 3.952$
Chromium	$10.370 \sqrt{A} - 3.125$
Copper	$11.138 \sqrt{A} - 10.918$
Iron	S
Lead	A
Magnesium	70.0
Manganese	S
Mercury	A
Nickel	$41.362 \ln(A) - 89.674$
Selenium	$9.738 \sqrt{A}$
Silver	$9.602 \sqrt{S}$
Thallium	——
Zinc	S
Uranium-238	$21.03 \ln (A + 1)$
Thorium-232	$21.03 \ln (A + 1)$
Radium-226	A
Radium-228	A
Lead-210	A

A = Percentage recovery of ash.
S = Percentage recovery of sulfur.

Output Vector of Clean Coal Characteristics. The quantity of each element appearing in the output clean coal vector is given by the following equation:

$$QO = 0.66\ QI - QSW + 0.34\ QI \text{ tons},$$

where

QO is the quantity in clean coal,

QI is the quantity in the input coal,

QSW is the quantity in the solid waste.

The total quantity of clean coal, calculated as the input amount less the dry total solid waste, is also given as a separate output.

Output Vector of Solid Waste

The solid waste consists of a wet >3/8-in. refuse and a <28-mesh slurry. The two waste streams may have different disposal requirements. The >3/8-in. refuse contains 6 to 12% moisture and can be disposed of in a landfill, whereas the <28 mesh slurry contains 15 to 25% moisture and may require separate ponding.[2]

The solid waste is therefore split into two output streams; 2.5% of which is assumed to be <28 mesh (from Reference 2) and contains 20% moisture, and the remainder to have a moisture content of 9%. All the elements are evenly divided between the two streams.

The total solid waste (element 25) is a wet weight and the total quantity of water (element 34) is also given. The other elements which compose the solid waste are given as dry quantities.

1.2.4 Level 3 Cleaning

The module assumes an overall Btu recovery of 85% (from Reference 2). In this case, all coal >28-mesh size is being cleaned and this constitutes 94% of the input coal (see Section 1.1.4). The Btu recovery for the coal subject to cleaning is 84%.

The same equations are used as for Level 2 cleaning to determine the amounts of the major and minor components of the solid waste. However, theremoval rates will be greater because of the greater Btu removal. Also, the equations are applied to 94% of the incoming coal.

Again, the solid waste is split into two streams to reflect the different moisture content. In this case the >3/8-in. streams constitute 65% of the solid waste and have a moisture content of 9%; the remainder is assumed to have a moisture content of 20%.

1.3 Computer Code

The computer code used is described in Appendix 1C. In Appendix 1D, there is a copy of the code along with a sample input and output.

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APPENDIX 1A

EQUATIONS FOR REMOVAL RATES OF MAJOR COAL COMPONENTS (CARBON, ASH, SULFUR) IN COAL CLEANING, LEVELS 2 AND 3

In determining equations for use in estimating the removal rates of various components of coal, certain assumptions had to be made in regard to which variables were directly related, and in what form. These assumptions were restricted by limited available data and the desire to keep the model as simple as possible. The following assumptions were made in constructing the coal cleaning module:

1. For each level (2 and 3) of coal cleaning, the Btu removal rate (BTUREM) is fixed.
2. PCWASTE = f(BTUREM, PCASH),

where

PCWASTE = % total coal removal,

PCASH = % ash content of the raw coal.

3. % removal of carbon = BTUREM.
4. Other elements in the raw coal not accounted for (mainly oxygen and nitrogen) = (total coal) - (carbon content) - (ash content) - (sulfur content).
5. % removal rate of other elements = BTUREM.
6. Amount of ash removed = (total coal removed) - (carbon removed) - (other removed).
7. % organic sulfur removal (ORGSREM) = BTUREM.
8. % pyritic sulfur removal (PCPSREM) = f(PCASHR, PCPYRS, PCWASTE, BTUREM),

where

PCPYRS = % pyritic sulfur content of the raw coal.

9. % removal of trace metals = f(PCASHR or PCPSREM) (see Appendix 1B).

After the above assumptions were made, data were obtained from Reference 3 for 455 coal samples which were subjected to float-sink washability studies. The clean coal used was the Float-1.6 fraction. This is the approximate specific gravity used in coal cleaning plants, as it gives the best tradeoff between the amount of coal recovered and the sulfur and ash removal.

The following variables were obtained or calculated from Reference 3:

1. % total coal removal (PCWASTE).
2. % total Btu removal (BTUREM).
3. % total ash content (PCASH).
4. % total pyritic sulfur content (PCPYRS).
5. % total ash removal (PCASHR).
6. % total pyritic sulfur removal (PCPSREM).

Because of analytical error, typographical error, or a coal sample which seemed extremely uncharacteristic in terms of one or more of its components, certain of the coal samples were eliminated before deriving the removal rate equations. After elimination, there were 441 coal samples available for use in the estimation of the equations.

Using the SPSS[11] regression program and the above assumptions, the following equations were obtained:

1. $\text{PCWASTE} = .719\ (\text{PCASH}) + .890\ (\text{BTUREM}) - 3.698 \qquad (R^2 = .92)$

2. $\text{PCPSREM} = .686\ (\text{PCASHR}) + 2.499\ (\text{BTUREM}) + 127.286\ (\text{Ln}(100-\text{PCWASTE}))$
   $+ 3.578\ (\text{Ln}(\text{PCPYRS})) - 584.565 \qquad (R^2 = .47)$

APPENDIX 1B

CALCULATION OF TRACE ELEMENT COEFFICIENTS

1B.1 Calculation of Fractionation Factors for Trace Elements

Using the results from the reports detailed in Section 1.2.3, the fraction of each trace element which appeared in the clean coal was calculated on a whole coal basis.

An example of how the data were converted to fractionation factors is given in Table 1B.1.

Table 1B.1
Example of Calculation of Fractionation Factor Using Results for Nickel

	Concentration ppm	Weight Fraction	Weighted Concentration	Weighted Concentration $\times \frac{11.0}{10.275}$
Float 1.29	8.0	0.343	2.744	2.938
Float 1.33	8.0	0.259	2.072	2.218
Float 1.40	10.0	0.186	1.860	1.991
Float 1.60	10.0	0.125	1.250	1.338
Sink 1.60	27.0	0.087	2.349	8.485
Composite		1.00	10.275	
Feed coal	11.0		11.00	

$$\text{Corrected concentration} = 8.485 \times \frac{100}{91.3} = 9.29 \ .$$

$$\text{Fractionation factor to clean coal} = \frac{9.29}{11.00} = 0.8449 \ .$$

The determined concentrations were multiplied by the weight fraction of the total coal found in each specific gravity zone to obtain the weighted concentration values. These values were "normalized" so that their summation totals the determined concentration of the feed (11.0 ppm in the example given). This was done by multiplying each of the weighted concentration values by the feed value (11.00), and dividing by 10.275, the summation of the weighted concentration values. The summation of these then equalled the feed value.

The total of these values for the "float" zones represents the weighted total concentration values in the four zones which are to represent the final cleaned coal. In this case these zones represented 91.3% of the total feed coal. To obtain the final concentration value for the cleaned coal, the value for 91.3% again had to be normalized to reflect 100%. This was done by multiplying the 8.485 by 100 and dividing by 91.3 to obtain 9.29 as concentration in the clean coal.

The fractionation factor is then determined by dividing 9.29 by the original concentration in the coal (11.0) to give a factor of 0.8449, which in this case represents the fraction of nickel remaining in the coal after washing.

Table 1B.2 gives the results and Table 1B.3 gives the key to the figures as to where the coal samples come from and which reference was used.

1B.2 Estimation of Trace Element Removal Rates

While it is acknowledged that removal of trace elements is not a simple function and is subject to large variation, an effort was made to make the estimation of removal rates as simple as possible. This was accomplished by assuming that the removal rate of each trace element is a function of the removal rate of either ash or pyritic sulfur.

The data for trace elements as described above were plotted vs the ash and pyritic sulfur data. (Note: the data above are expressed in terms of fraction recovery rate, i.e., the proportion of the component which ends up in

Table 1B.2
Trace Metal Coal Cleaning Data
Fraction to Clean Coal

Element	S1 3/8"x28m	S2 3/8"x28m	S3 3/8"x28m	S4 3/8"x28m	S5 3/8"x28m	S6 3/8"x28m	S7 3/8"x28m	S8 3/8"x0	S9 3/8"x0	S10 3/8"x0	S11 3/8"x0	S12 3/8"x0	S13 3/8"x0	S14 3/8"x0	S15 3/8"x0
Ash	0.6815	0.7052	0.5023	0.7176				0.75	0.65	0.37	0.60	0.67	0.93	0.92	0.47
Btu	1.0630	1.0384	1.0760	1.0367				1.02	1.12	1.31	1.14	1.07	1.02	1.02	1.19
Sulfur pyritic	0.4088	0.7547	0.3878	0.8757	0.2376	0.5101	0.3759	0.71	0.33	0.44	0.63	0.85	0.79	0.90	0.83
Sulfur total	0.7002	0.9850	0.8566	0.9673	0.4568	0.6352	0.6522	0.76	0.44	0.55	0.74	0.91	0.82	0.93	0.89
Antimony	0.8155	0.8425	0.8573	0.8187	0.8905	0.9441	0.7361								
Arsenic	0.3391	0.5302	0.2888	0.8188	0.3051	0.5069	0.1880	0.79	0.33	0.33	0.41	0.85	0.61	0.89	0.55
Beryllium	0.7184	0.4996	0.8699	0.9565	1.0320	0.9185	0.9739	1.03	0.90	0.83	0.92	1.04	1.01	1.02	0.72
Cadmium	0.5195	0.7435	0.8182	0.8861	0.1048	0.0298	0.6383	0.79							
Chromium	0.8344	0.8385	0.6944	0.6874	0.9221	0.3837	0.6144	0.96	0.78	0.60	0.74	0.85	0.99	0.98	0.74
Copper	0.8684	0.9266	0.8314	0.7276	0.8987	0.7202	0.5116	0.97	0.56	0.44	0.75	0.88	0.92	0.92	0.70
Iron	0.4997	0.7464	0.8207	0.8408	0.3840	0.5971	0.3857	0.64	0.35	0.42	0.60	0.76	0.78	0.87	0.74
Lead	0.6921	0.9048	0.7250	0.9428	0.2507	0.8104	0.2187	0.72	0.47	0.37	0.63	0.92	0.81	0.84	0.66
Magnesium	0.7711	0.5308	0.6685	0.7259	0.7242		0.3090								
Manganese	0.5011	0.4762	0.7289	0.7633	0.6701	0.3554	0.1661	0.84	0.47	0.24	0.42	0.61	0.91	0.76	0.82
Mercury	0.8614	0.9858	0.5447	0.9267	0.3585	0.7077	0.4820	0.77	0.36	0.32	0.56	0.97	0.85	0.96	0.80
Nickel	0.8449	0.9914	0.9586	0.9404	0.8457	0.7947	0.5629	0.92	0.64	0.45	0.80	0.79	0.92	0.97	0.77
Selenium	0.7683	0.9038	0.7481	0.8396	0.8267	0.8808	0.5934	0.91	0.39	0.45	0.61	0.81	0.90	0.98	0.71
Silver	0.7135	0.8686	0.4824	0.8758											
Thallium															
Zinc	0.3137	0.7399	0.8626	0.8125	0.1829	0.0258	0.0242	0.57	0.59	0.61	0.66	0.87	0.72	0.83	0.54
Uranium	0.9213	0.9074	0.7684	0.9107											
Thorium	0.8587	0.7482	0.6994	0.6561											

Table 1B.2 (cont.)
Fraction to Clean Coal

Element	S16 14 mesh x0	S17 14 mesh x0	S18 14 mesh x0	S19 14 mesh x0	S20 14 mesh x0	S21 14 mesh x0	S22 14 mesh x0	S23 3/8"x0	S24 3/8"x0	S25 14 mesh x0	S26 14 mesh x0	S27 14 mesh x0	S28 14 mesh x0	S29 14 mesh x0
Ash														
Btu														
Sulfur pyritic														
Sulfur total														
Antimony														
Arsenic														
Beryllium														
Cadmium	0.7980	0.7264	0.7585	0.9805	0.0276	0.1521	0.6118	0.9203	0.5219	0.8338		1.0490		
Chromium	0.8806	0.9146	0.7087	0.4182	0.8788	1.0317	0.9163	0.9271	1.0670	0.8712	0.4184	0.4184		
Copper	0.7555	0.5661	0.5705	0.6687	0.6564	0.8866	0.8661	0.9101	0.8344	0.9578	0.6689	0.6689		
Iron														
Lead	0.7138	0.4690	0.3361	0.4988	0.5872	0.9304	0.7225	0.8523	0.6873	0.8886		0.5151		
Magnesium														
Manganese	0.3782	0.5259	0.4968	0.2234	0.3140	0.1709	0.8204	0.9652	0.2781	0.3286	0.2484	0.2484		
Mercury	0.5450	0.5796	0.5402	0.5993	0.8922	0.9497	0.7625	0.9396	0.6025	0.9299	0.5402		0.5402	0.7216
Nickel	0.8829	0.6715	0.7194	0.7003	0.9057	1.0617	0.9872	1.0080	0.6049	0.6564	0.7006	0.7006		
Selenium														
Silver														
Thallium														
Zinc														
Uranium														
Thorium														

Table 1E.3
Key to Trace Metal Factors

No.	Reference	Coal Sample
S1	7	Illinois Herrin No. 6
S2	7	Alabama Blue Creek
S3	7	W. Virginia Pocahontas No. 4
S4	7	W. Virginia Pittsburgh No. 8
S5	7	Illinois Davis
S6	7	Illinois Colchester No. 2
S7	7	Illinois Herrin No. 6
S8	8	W. Kentucky No. 6 Seam, Butler Co., KY
S9	8	Bakerstown Seam, Grant Co., WV
S10	8	Lower Kittanning Seam, Westmoreland Co., PA
S11	8	Lower Freeport Seam, Indiana Co., PA
S12	8	Ft. Scott Seam, Rogers Co., OK
S13	8	Lower Freeport Seam, Butler Co., PA
S14	8	Baxter Seam, Crawford Co., KS
S15	8	Clements Seam, Walker Co., AL
S16	9	Pittsburgh coalbed, PA
S17	9	Waynesburg coalbed, OH
S18	9	Upper Freeport coalbed, MD
S19	9	Hazard No. 4 coalbed, KY (East)
S20	9	No. 6 coalbed, IL
S21	9	No. 5 coalbed, IL
S22	9	No. 7 coalbed, KY (West)
S23	9	Red coalbed, AZ
S24	9	No. 8 coalbed, NM
S25	9	Rock Springs No. 3 coalbed, WY
S26	10	Upper Freeport coalbed Garett Co., MD
S27	10	Hazard No. 4 Bell Co., KY
S28	10	Indiana V coalbed, Pike Co., IN
S29	10	Lower Kittanning coalbed, Centre Co., MD

the clean coal. The functions derived below are given in terms of percentage recovery rate, 100 x (proportion recovered). The fraction removal rate as calculated in the computer module is determined by

$$F(E) = (100 - R(E))/100,$$

where

$F(E)$ = fraction removal of trace element E,

$R(E)$ = percent recovery rate of trace element E,

and R(E) for all trace elements are described below. The data supplied between four and twelve points per graph.

The graphs were then compared to sample graphs which showed the form for the linear, log, and square root functions. The best form for each element was chosen, and a line was fitted for each element according to Table 1.B4, using least squares regression. In some cases, data points which seemed to be outliers were eliminated before fitting a line (See comments, Table 1B.4). Some of the trace elements showed no pattern, but were grouped around a certain recovery rate, and were therefore assigned a constant (average) recovery rate.

Table 1B.4

Trace Element Recovery as a Function of Ash or Pyritic Sulfur Recovery

Trace Element	Functional Form*	Equation**	Comments
Antimony	Average	$R = 85.0$	Deleted S_6,S_7 (max and min values)
Arsenic	Linear (A)	$R = A$	-
Beryllium	Sq. root (A)	$R = 4.641\sqrt{A}+49.713$	
Cadmium	Exponential(S)	$Ln(R) = .006S+3.952$	Deleted S_5,S_6
Chromium	Sq. root (A)	$R = 10.370\sqrt{A}-3.125$	-
Copper	" " "	$R = 11.138\sqrt{A}-10.918$	-
Iron	Linear (S)	$R = S$	-
Lead	Linear (A)	$R = A$	Assumed Pb^{210} rate is same as lead
Magnesium	Average	$R = 70.0$	Used approximate mode
Manganese	Linear (S)	$R = S$	-
Mercury	Linear (A)	$R = A$	Regression line, when forced through origin, is $R = 1.106\ A$
Nickel	Log (A)	$R = 41.362\ Ln(A) -89.674$	-
Selenium	Sq. root (A)	$R = 9.738\ \sqrt{A}$	Deleted S_9, forced line through origin
Silver	Sq. root (S)	$R = 9.602\ \sqrt{S}$	Forced line through origin
Thallium	-	-	No data available, set=0
Zinc	Linear (S)	$R = S$	-
Uranium and Thorium	Log (A)	$R = 21.03\ Ln(A+1)$	Line estimated using uranium data and forced through origin
Radium-226 and Radium-228	Linear (A)	$R = A$	-
Lead-210	Linear (A)	$R = A$	Assumed same rates as lead

* Functional form given as F(X) where F is the function and
$X =$ A (ash recovery rate) or,
S (pyritic sulfur recovery rate).

** R = trace element recovery rate,
A = ash recovery rate,
S = pyritic sulfur recovery rate.

APPENDIX 1C

DESCRIPTION OF COMPUTER MODULE

The computer module for the coal cleaning process consists of four subroutines (CLEAN, TRACE, STRSPL, CPRINT). The module is operated by making a call to CLEAN,

Call CLEAN (Q, LEVEL, COAL),

where

Q = total amount of coal.

LEVEL = integer value, indicates the level of coal cleaning desired. Acceptable values of LEVEL are 1, 2, or 3. Any other value will immediately return control to the calling program.

COAL = input vector of coal characteristics, dimension 50. On output it will contain the characteristics of the cleaned coal.

For LEVEL 1 cleaning (sizing), CLEAN will calculate all output characteristics directly. For other levels, it will set the Btu removal rate, the coal split for the cleaned and passed-through coal, and the split for the two solid waste output streams and calculate the percentage of ash and pyritic sulfur in the coal. It will then call subroutines TRACE and STRSPL to calculate the major component and trace metal removal rates and the solid waste split, respectively.

After the characteristics of the solid waste are determined, subroutine CPRINT is called to print out all input and output vectors.

Subroutine TRACE

Using the Btu removal rate and the ash and pyritic sulfur content from subroutine CLEAN, the solid waste characteristics are calculated in TRACE as shown in Appendix 1A (ash, carbon, sulfur) and Appendix 1B (trace metals). The solid waste characteristics are placed in vector STREAM1.

The removal rates of all components, which were in percentages, are converted to proportions. Control is returned to subroutine CLEAN.

Subroutine STRSPL

After cleaning at level 2 or 3, the solid waste is split into two streams for different levels of disposal. STRSPL converts the output solid waste calculated in TRACE to two output waste streams (which will contain water).

Subroutine CPRINT

Subroutine CPRINT prints out the input and output vectors used in the module. For each element, output consists of:

1. Fraction removed - this fraction is the fraction removed of only the coal which is cleaned (all for Level 1, appropriate amounts for 2 and 3).
2. Input coal components.
3. Clean coal components.
4. STREAM1 and STREAM2 - solid waste streams as determined for levels 2 and 3. For Level 1, STREAM1 will contain all of the solid waste, STREAM2 will be a zero vector.

Special notes:

1. If the Ra^{226}, Ra^{228} and Pb^{210} elements of the input coal are zero, they will be calculated from uranium and thorium (see Section 7) upon calling CLEAN even if LEVEL is a value other than 1, 2, or 3.

2. The input coal vector is saved in vector OCOAL within the subroutine CPRINT.

3. For Levels 2 and 3, a certain proportion of the coal is cleaned and a certain proportion is passed through to the output coal. After part is cleaned (by calls to subroutines TRACE and STRSPL), the cleaned and passed-through coal vectors are added together to give the characteristics of the total cleaned coal.

4. Common block REM (dimension 24) is used in storing removal rates which are printed in CPRINT.

5. Fraction of total sulfur removed on output is the fraction of organic sulfur removed, while all other values of total sulfur are of total sulfur (organic and pyritic). Total sulfur removed is calculated by

   Organic sulfur content = Total sulfur content - pyritic sulfur content.

   Total sulfur removed = (fraction organic sulfur removed) x (organic sulfur content) + (fraction pyritic sulfur removed) x (pyritic sulfur content)

6. Empty vector elements which are not used or are not applicable to the coal cleaning process are set to zero but are not printed.

7. No data were available for calculating fraction removed of thallium in Levels 2 and 3, and are set at zero.

8. Fraction removed of total solid waste is the fraction of the total coal removed by weight.

APPENDIX 1D

COMPUTER CODE AND SAMPLE OUTPUT

This appendix sets out the computer code used for the coal-cleaning module with a sample input and the resulting output. Table 1D.1 gives the coal characteristics used as input. The other input variables used were as follows:

Quantity of coal (Q) = 100,000.0 tons,

Level of cleaning (LEVEL) = 2.

For total sulfur (element 2) the fraction removed in fact applies to organic sulfur only, although the rest of the vectors give the data for total sulfur (pyritic and organic).

Table 1D.1
Input Characteristics of Coal

Element	Input Quantity (tons)
Ash	18700.00
Sulfur	3000.00
Antimony	0.07
Arsenic	2.70
Beryllium	0.50
Cadmium	0.125
Chromium	3.00
Copper	1.18
Iron	2700.00
Lead	1.14
Magnesium	118.00
Manganese	7.40
Mercury	0.017
Nickel	2.00
Selenium	0.02
Silver	0.01
Zinc	1.69
Uranium	0.07
Thorium	0.66
Pyritic sulfur	1870.00
Carbon	64100.00
Btu	2.3E12

```
      PROGRAM CLL(OUTPUT,TAPE2=OUTPUT)
      DIMENSION COAL(50)
      Q=100000
      COAL(1)=18700.
      COAL(2)=3000.
      COAL(3)=.07
      COAL(4)=2.7
      COAL(5)=.5
      COAL(6)=.125
      COAL(7)=3.
      COAL(8)=1.18
      COAL(9)=2700
      COAL(10)=1.14
      COAL(11)=118.
      COAL(12)=7.4
      COAL(13)=.017
      COAL(14)=2.
      COAL(15)=.02
      COAL(16)=.01
      COAL(17)=0.
      COAL(18)=1.69
      COAL(19)=.07
      COAL(20)=.66
      DO 10 I=21,38
      COAL(I)=0.
   10 CONTINUE
      COAL(39)=1870.
      COAL(40)=64100
      COAL(41)=2.3E12
      DO 20 I=42,50
      COAL(I)=0.
   20 CONTINUE
      COAL(17)=1.
      LEVEL=2
      CALL CLEAN(Q,LEVEL,COAL)
      STOP
      END
```

```
      SUBROUTINE CLEAN(Q,LEVEL,COAL)
      DIMENSION COAL(50),SCOAL(50),STREAM1(50),STREAM2(50),OCOAL(50)
      COMMON/REM/REMOV(24)
C   * CALCULATION OF INPUT RA-226,RA-228 & PB-210 IF NOT GIVEN
      IF(COAL(21) .EQ. 0.)COAL(21)=3.38E-7*COAL(19)
      IF(COAL(22) .EQ. 0.)COAL(22)=4.01E-10*COAL(20)
      IF(COAL(23) .EQ. 0.)COAL(23)=4.37E-9*COAL(19)
      DO 1 I=1,50
C   * OCOAL USED TO STORE INPUT CHARACTERISTICS FOR PRINT OUT
      OCOAL(I)=COAL(I)
    1 CONTINUE
      IF(LEVEL .EQ. 3)GO TO 100
      IF(LEVEL .EQ. 2)GO TO 100
C   * LEVEL MUST BE AN INTEGER BETWEEN 1 AND 3
      IF(LEVEL .NE. 1)GO TO 5000
C   * CALCULATION OF WASTE FROM LEVEL 1 CLEANING
C   * CALCULATION OF FRACTION OF INCOMING ASH REMOVED
      POTHER=(.02*Q-.005*COAL(40))/(Q-COAL(40))
C   * CALCULATION OF INPUT AMOUNT OF ORGANIC SULFUR
      ORGS=COAL(2)-COAL(39)
C   * CALCULATION OF AMOUNT OF ORGANIC SULFUR REMOVED
      ORGSREM=.005*ORGS
C   * CALCULATION OF ASH IN WASTE AND CLEAN COAL
      STREAM1(1)=POTHER*COAL(1)
      COAL(1)=COAL(1)-STREAM1(1)
C   * CALCULATION OF TRACE ELEMENT SPLIT BETWEEN WASTE AND CLEAN COAL
      DO 10 I=3,24
      STREAM1(I)=POTHER*COAL(I)
      COAL(I)=COAL(I)-STREAM1(I)
   10 CONTINUE
C   * CALCULATION OF WATER CONTENT OF SOLID WASTE
      STREAM1(25)=.02*Q
C   * NON-APPLICABLE ELEMENTS SET TO ZERO
      DO 20 I=26,38
      STREAM1(I)=0.
   20 CONTINUE
C   * CALCULATION OF PYRITIC SULFUR SPLIT BETWEEN WASTE AND CLEAN COAL
      STREAM1(39)=POTHER*COAL(39)
      COAL(39)=COAL(39)-STREAM1(39)
C   * CALCULATION OF TOTAL SULFUR SPLIT BETWEEN WASTE AND CLEAN COAL
      STREAM1(2)=STREAM1(39)+ORGSREM
      COAL(2)=COAL(2)-STREAM1(2)
C   * SPLIT OF CARBON AND BTUS BETWEEN WASTE AND CLEAN COAL
      STREAM1(40)=.005*COAL(40)
      STREAM1(41)=.005*COAL(41)
      COAL(40)=COAL(40)-STREAM1(40)
      COAL(41)=COAL(41)-STREAM1(41)
      DO 30 I=42,50
C   * NON-APPLICABLE ELEMENTS SET TO ZERO
      STREAM1(I)=0.
   30 CONTINUE
C   * LEVEL 1 CLEANING HAS ONLY ONE OUTPUT WASTE STREAM
      DO 40 I=1,50
      STREAM2(I)=0.
   40 CONTINUE
C   * QUANTITY OF CLEAN COAL CALCULATED
      QCLEAN=Q-STREAM1(25)
C   * FRACTION OF EACH ELEMENT REMOVED CALCULATED FOR PRINTOUT
      REMOV(1)=.02
      REMOV(2)=POTHER
      REMOV(3)=.005
      DO 50 I=4,24
      REMOV(I)=POTHER
```

```
   50 CONTINUE
      BTUREM=.005
      GO TO 500
C   * CALCULATION OF WASTE FROM LEVEL 2 AND 3 CLEANING
C
C   * BTU REMOVAL PERCENTAGE SET FOR LEVELS 2 AND 3
  100 IF(LEVEL .EQ. 2)BTUREM=10.6
      IF(LEVEL .EQ. 3)BTUREM=16.0
C   * LEVEL 2 CLEANING 34% OF INPUT COAL NOT CLEANED
C   * LEVEL 3 CLEANING 6% OF INPUT COAL NOT CLEANED
      IF(LEVEL .EQ. 2)SPLIT=.34
      IF(LEVEL .EQ. 3)SPLIT=.06
C   * LEVEL 2  WASTE STREAMS SPLIT 97.5% AND 2.5%
C   * LEVEL 3 WASTE STREAMS SPLIT 65% AND 35%
      IF(LEVEL .EQ. 2)S2SPLIT=.025
      IF(LEVEL .EQ. 3)S2SPLIT=.350
C   * CALCULATION OF PERCENTAGE OF ASH AND PYRITIC SULFUR IN INPUT COAL
      PCASH=100.*COAL(1)/Q
      PCPYRS=100.*COAL(39)/Q
C   * INPUT ELEMENTS SPLIT BETWEEN COAL NOT SUBJECT TO CLEANING AND
C   * COAL SUBJECT TO CLEANING
      DO 110 I=1,24
      SCOAL(I)=SPLIT*COAL(I)
      COAL(I)=COAL(I)-SCOAL(I)
  110 CONTINUE
      DO 120 I=39,41
      SCOAL(I)=SPLIT*COAL(I)
      COAL(I)=COAL(I)-SCOAL(I)
  120 CONTINUE
C   * CALCULATION OF QUANTITY OF COAL SUBJECT TO CLEANING
      QSPLIT=Q-SPLIT*Q
      CALL TRACE(QSPLIT,BTUREM,PCASH,PCPYRS,COAL,STREAM1)
      CALL STRSPL(S2SPLIT,STREAM1,STREAM2)
C   * CALCULATION OF TOTAL QUANTITY OF EACH ELEMENT IN OUTPUT COAL
C   * - ELEMENT IN CLEAN COAL + ELEMENT IN COAL NOT SUBJECT TO CLEANING
      DO 130 I=1,24
      COAL(I)=COAL(I)+SCOAL(I)
  130 CONTINUE
      DO 140 I=39,41
      COAL(I)=COAL(I)+SCOAL(I)
  140 CONTINUE
C   * CALCULATION OF TOTAL OUTPUT QUANTITY OF COAL
      QCLEAN=QSPLIT+SPLIT*Q
  500 CALL CPRINT(Q,QCLEAN,BTUREM,COAL,STREAM1,STREAM2,QCOAL)
 5000 RETURN
      END
```

```
      SUBROUTINE TRACE(Q,BTUREM,PCASH,PCPYRS,COAL,STREAM1)
C   * USED TO CALCULATE THE SPLIT BETWEEN WASTE AND CLEAN COAL
C   * FOR EACH ELEMENT
      DIMENSION COAL(50),STREAM1(50)
      REAL SBREC,SBREM,ASREC,ASREM,BEREC,BEREM,CDREC,CDREM,
     -CRREC,CRREM,CUREC,CUREM,FEREM,PBREM,MGREC,MGREM,MNREM,
     -NIREC,NIREM,HGREM,SEREC,SEREM,AGREC,AGREM,ZNREM,UREC,UREM,
     -THREM,PB210R
      COMMON/REM/PCWASTE,PCASHR,PCOSREM,SBREM,ASREM,BEREM,CDREM,CRREM,
     -CUREM,FEREM,PBREM,MGREM,MNREM,HGREM,NIREM,SEREM,AGREM,
     -ZNREM,UREM,THREM,RAREM,PB210R,PCPSREM,TLREM
C   * CALCULATION OF PERCENTAGE OF INPUT COAL REMOVED AS WASTE
      PCWASTE=.719*PCASH+.890*BTUREM-3.698
C   * CALCULATION OF TOTAL DRY WASTE
      WASTE=PCWASTE*Q/100.
C   * CALCULATION OF AMOUNT OF CARBON REMOVED
      CREM=BTUREM*COAL(40)/100.
C   * CALCULATION OF O,N AND H IN COAL
      OXNIT=Q-COAL(1)-COAL(2)-COAL(40)
C   * CALCULATION OF ASH CONTENT OF WASTE
      ASHREM=WASTE-CREM-BTUREM*OXNIT/100.
C   * CALCULATION OF INPUT ORGANIC SULFUR
      ORGS=COAL(2)-COAL(39)
C   * CALCULATION OF PERCENTAGE OF ASH REMOVED
      PCASHR=100.*ASHREM/COAL(1)
C   * CALCULATION OF PERCENTAGE OF PYRITIC SULFUR REMOVED
      PCPSREM=.686*PCASHR+2.499*BTUREM+127.286*ALOG(100.-PCWASTE)
     - +3.578*ALOG(PCPYRS)-584.565
C   * CALCULATION OF QUANTITY OF EACH ELEMENT IN WASTE AND CLEAN COAL
C   * VARIABLE NAMES ENDING IN 'RC'  REFER TO % RECOVERED IN CLEAN
C   * COAL AND 'REM' REFERS TO % REMOVED
C
C     ASH
C
      PCASHRC=100.-PCASHR
      STREAM1(1)=PCASHR*COAL(1)/100.
      COAL(1)=COAL(1)-STREAM1(1)
C
C     INORGANIC (PYRITIC) SULFUR
C
      PCPSRC=100.-PCPSREM
      STREAM1(39)=PCPSREM*COAL(39)/100.
      COAL(39)=COAL(39)-STREAM1(39)
C
C     TOTAL SULFUR
C
      ORGSREM=BTUREM*ORGS/100.
      PCOSREM=ORGSREM/ORGS
      STREAM1(2)=STREAM1(39)+ORGSREM
      COAL(2)=COAL(2)-STREAM1(2)
C
C     CARBON AND BTU
C
      STREAM1(40)=BTUREM*COAL(40)/100.
      COAL(40)=COAL(40)-STREAM1(40)
      COAL(41)=COAL(41)-BTUREM*COAL(41)/100.
      STREAM1(41)=0.
C
C     ANTIMONY
C
      SBREC=85.0
      SBREM=(100.-SBREC)/100.
      STREAM1(3)=SBREM*COAL(3)
```

```
      COAL(3)=COAL(3)-STREAM1(3)
C
C     ARSENIC
C
      ASREC=PCASHRC
      ASREM=(100.-ASREC)/100.
      STREAM1(4)=ASREM*COAL(4)
      COAL(4)=COAL(4)-STREAM1(4)
C
C     BERYLLIUM
C
      BEREC=49.713+4.641*SQRT(PCASHRC)
      BEREM=(100.-BEREC)/100.
      STREAM1(5)=BEREM*COAL(5)
      COAL(5)=COAL(5)-STREAM1(5)
C
C     CADMIUM
C
      CDREC=.006*PCPSRC+3.952
      CDREC=EXP(CDREC)
      CDREM=(100.-CDREC)/100.
      STREAM1(6)=CDREM*COAL(6)
      COAL(6)=COAL(6)-STREAM1(6)
C
C     CHROMIUM
C
      CRREC=10.370*SQRT(PCASHRC)-3.125
      CRREM=(100.-CRREC)/100.
      STREAM1(7)=CRREM*COAL(7)
      COAL(7)=COAL(7)-STREAM1(7)
C
C     COPPER
C
      CUREC=11.138*SQRT(PCASHRC)-10.918
      CUREM=(100.-CUREC)/100.
      STREAM1(8)=CUREM*COAL(8)
      COAL(8)=COAL(8)-STREAM1(8)
C
C     IRON
C
      FEREM=PCPSREM/100.
      STREAM1(9)=FEREM*COAL(9)
      COAL(9)=COAL(9)-STREAM1(9)
C
C     LEAD
C
      PBREM=PCASHR/100.
      STREAM1(10)=PBREM*COAL(10)
      COAL(10)=COAL(10)-STREAM1(10)
C
C     MAGNESIUM
C
      MGREC=70.0
      MGREM=(100.-MGREC)/100.
      STREAM1(11)=MGREM*COAL(11)
      COAL(11)=COAL(11)-STREAM1(11)
C
C     MANGANESE
C
      MNREM=PCPSREM/100.
      STREAM1(12)=MNREM*COAL(12)
      COAL(12)=COAL(12)-STREAM1(12)
C
```

```
C     MERCURY
C
      HGREM=PCASHR/100.
      STREAM1(13)=HGREM*COAL(13)
      COAL(13)=COAL(13)-STREAM1(13)
C
C     NICKEL
C
      NIREC=41.362*ALOG(PCASHRC)-89.674
      NIREM=(100.-NIREC)/100.
      STREAM1(14)=NIREM*COAL(14)
      COAL(14)=COAL(14)-STREAM1(14)
C
C     SELENIUM
C
      SEREC=9.738*SQRT(PCASHRC)
      SEREM=(100.-SEREC)/100.
      STREAM1(15)=SEREM*COAL(15)
      COAL(15)=COAL(15)-STREAM1(15)
C
C     SILVER
C
      AGREC=9.602*SQRT(PCPSRC)
      AGREM=(100.-AGREC)/100.
      STREAM1(16)=AGREM*COAL(16)
      COAL(16)=COAL(16)-STREAM1(16)
C
C     ZINC
C
      ZNREM=PCPSREM/100.
      STREAM1(18)=ZNREM*COAL(18)
      COAL(18)=COAL(18)-STREAM1(18)
C
C     URANIUM
C
      UREC=21.03*ALOG(PCASHRC+1)
      UREM=(100.-UREC)/100.
      STREAM1(19)=UREM*COAL(19)
      COAL(19)=COAL(19)-STREAM1(19)
C
C     THORIUM
C
      THREM=UREM
      STREAM1(20)=THREM*COAL(20)
      COAL(20)=COAL(20)-STREAM1(20)
C
C     RADIUM-226 AND RADIUM-228
C
      RAREM=PCASHR/100.
      STREAM1(21)=RAREM*COAL(21)
      STREAM1(22)=RAREM*COAL(22)
      COAL(21)=COAL(21)-STREAM1(21)
      COAL(22)=COAL(22)-STREAM1(22)
C
C     LEAD-210
C
      PB210R=PBREM
      STREAM1(23)=PB210R*COAL(23)
      COAL(23)=COAL(23)-STREAM1(23)
C
C     TOTAL WASTE
C
      STREAM1(25)=STREAM1(1)+STREAM1(40)
```

```
C     OTHERS (UNKNOWN AND NOT APPLICABLE)
C
      TLREM=0.
      STREAM1(17)=0.
      STREAM1(24)=0.
      DO 10 I=26,38
      STREAM1(I)=0.
   10 CONTINUE
      DO 20 I=42,50
      STREAM1(I)=0.
   20 CONTINUE
C   * PERCENTAGE REMOVALS CONVERTED TO FRACTIONS FOR PRINT OUT
      PCASHR=PCASHR/100.
      BTUREM=BTUREM/100.
      PCPSREM=PCPSREM/100.
      PCWASTE=PCWASTE/100.
C   * CALCULATION OF QUANTITY OF CLEAN COAL
      Q=Q-PCWASTE*Q
      RETURN$END


      SUBROUTINE STRSPL(S2SPLIT,STREAM1,STREAM2)
C   * SPLITS WASTE INTO TWO STREAMS TO REFLECT DIFFERENT DISPOSAL PRACTISES
      DIMENSION STREAM1(50),STREAM2(50)
      DO 10 I=1,50
C   * ALL ELEMENTS SPLIT INTO  2 WASTE STREAMS, FRACTIONAL SPLIT
C   * (S2SPLIT) DEFINED IN SUBROUTINE CLEAN
      STREAM2(I)=S2SPLIT*STREAM1(I)
      STREAM1(I)=STREAM1(I)-STREAM2(I)
   10 CONTINUE
C   * CALCULATION OF WATER CONTENT OF THE 2 WASTE STREAMS
      STREAM1(34)=.09*STREAM1(25)
      STREAM2(34)=.20*STREAM2(25)
C   * CALCULATION OF THE TOTAL WET WEIGHT OF THE 2 WASTE STREAMS
      STREAM1(25)=STREAM1(25)+STREAM1(34)
      STREAM2(25)=STREAM2(25)+STREAM2(34)
      RETURN$END


      SUBROUTINE CPRINT(Q,QCLEAN,BTUREM,COAL,STREAM1,STREAM2,OCOAL)
      DIMENSION COAL(50),STREAM1(50),STREAM2(50),OCOAL(50)
      COMMON/REM/PCWASTE,PCASHR,ORGSREM,SBREM,ASREM,BEREM,CDREM,CRREM,
     -CUREM,FEREM,PBREM,MGREM,MNREM,HGREM,NIREM,SEREM,AGREM,
     -ZNREM,UREM,THREM,RAREM,PB210R,PCPSREM,TLREM
      REAL SBREM,ASREM,BEREM,CDREM,CRREM,CUREM,FEREM,PBREM,MGREM,MNREM,
     -HGREM,NIREM,SEREM,AGREM,ZNREM,UREM,THREM,PB210R
      WRITE(2,2001)Q,PCWASTE,QCLEAN
 2001 FORMAT(1X,*TOTAL INPUT COAL:*,1X,E12.5/
     -10X,*FRACTION COAL REMOVAL:*,1X,F6.4,10X,*TOTAL CLEAN COAL*
     -,1X,E12.5)
      WRITE(2,2002)
 2002 FORMAT(1X,*CONSTITUENT*,T20,*FRACTION REMOVED*,T40,*INPUT COAL*,
     -T60,*CLEAN COAL*,T80,*STREAM1*,T100,*STREAM2*/
     -1X,11(*-*),T20,16(*-*),T40,10(*-*),T60,10(*-*),T80,
     -7(*-*),T100,7(*-*)/)
      WRITE(2,2004)PCASHR,OCOAL(1),COAL(1),STREAM1(1),STREAM2(1),
     -ORGSREM,OCOAL(2),COAL(2),STREAM1(2),STREAM2(2),
     -SBREM,OCOAL(3),COAL(3),STREAM1(3),STREAM2(3),
     -ASREM,OCOAL(4),COAL(4),STREAM1(4),STREAM2(4)
```

```
2004 FORMAT(1X,*ASH*,T20,E12.5,T40,E12.5,T60,E12.5,T80,E12.5,
    -T100,E12.5/1X,*TOTAL SULFUR*,T20,E12.5,T40,E12.5,T60,E12.5,
    -T80,E12.5,T100,E12.5/1X,*ANTIMONY*,T20,E12.5,
    -T40,E12.5,T60,E12.5,T80,E12.5,T100,E12.5/
    -1X,*ARSENIC*,T20,E12.5,T40,E12.5,T60,E12.5,T80,E12.5,T100,E12.5
    -)
     WRITE(2,2005)BEREM,OCOAL(5),COAL(5),STREAM1(5),STREAM2(5),
    -CDREM,OCOAL(6),COAL(6),STREAM1(6),STREAM2(6),
    -CRREM,OCOAL(7),COAL(7),STREAM1(7),STREAM2(7),
    -CUREM,OCOAL(8),COAL(8),STREAM1(8),STREAM2(8)
2005 FORMAT(1X,*BERYLLIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*CADMIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*CHROMIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*COPPER*,T20,E12.5,4(8X,E12.5))
     WRITE(2,2006)FEREM,OCOAL(9),COAL(9),STREAM1(9),STREAM2(9),
    -PBREM,OCOAL(10),COAL(10),STREAM1(10),STREAM2(10),
    -MGREM,OCOAL(11),COAL(11),STREAM1(11),STREAM2(11),
    -MNREM,OCOAL(12),COAL(12),STREAM1(12),STREAM2(12)
2006 FORMAT(1X,*IRON*,T20,E12.5,4(8X,E12.5)/
    -1X,*LEAD*,T20,E12.5,4(8X,E12.5)/
    -1X,*MAGNESIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*MANGANESE*,T20,E12.5,4(8X,E12.5))
     WRITE(2,2007)HGREM,OCOAL(13),COAL(13),STREAM1(13),STREAM2(13),
    -NIREM,OCOAL(14),COAL(14),STREAM1(14),STREAM2(14),
    -SEREM,OCOAL(15),COAL(15),STREAM1(15),STREAM2(15),
    -AGREM,OCOAL(16),COAL(16),STREAM1(16),STREAM2(16)
2007 FORMAT(1X,*MERCURY*,T20,E12.5,4(8X,E12.5)/
    -1X,*NICKEL*,T20,E12.5,4(8X,E12.5)/
    -1X,*SELENIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*SILVER*,T20,E12.5,4(8X,E12.5))
     WRITE(2,2018)TLREM,OCOAL(17),COAL(17),STREAM1(17),STREAM2(17),
    -ZNREM,OCOAL(18),COAL(18),STREAM1(18),STREAM2(18),
    -UREM,OCOAL(19),COAL(19),STREAM1(19),STREAM2(19),
    -THREM,OCOAL(20),COAL(20),STREAM1(20),STREAM2(20)
2018 FORMAT(1X,*THALLIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*ZINC*,T20,E12.5,4(8X,E12.5)/
    -1X,*URANIUM*,T20,E12.5,4(8X,E12.5)/
    -1X,*THORIUM*,T20,E12.5,4(8X,E12.5))
     WRITE(2,2008)RAREM,OCOAL(21),COAL(21),STREAM1(21),STREAM2(21),
    -RAREM,OCOAL(22),COAL(22),STREAM1(22),STREAM2(22),
    -PB210R,OCOAL(23),COAL(23),STREAM1(23),STREAM2(23),
    -OCOAL(24),COAL(24),STREAM1(24),STREAM2(24)
2008 FORMAT(1X,*RADIUM-226*,T20,E12.5,4(8X,E12.5)/
    -1X,*RADIUM-228*,T20,E12.5,4(8X,E12.5)/
    -1X,*LEAD-210*,T20,E12.5,4(8X,E12.5)/
    -1X,*HYDROCARBONS*,T40,E12.5,3(8X,E12.5))
     WRITE(2,2009)PCWASTE,OCOAL(25),COAL(25),STREAM1(25),STREAM2(25)
2009 FORMAT(1X,*TOTAL SOLID WASTE*,T20,E12.5,4(8X,E12.5))
     J=0
C    WRITE(2,2010)(J,OCOAL(I),COAL(I),STREAM1(I),STREAM2(I),I=26,33)
2010 FORMAT(I1,*NOT APPLICABLE*.T20,E12.5,4(8X,E12.5))
     WRITE(2,2011)OCOAL(34),COAL(34),STREAM1(34),STREAM2(34)
2011 FORMAT(1X,*WATER*,T40,E12.5,3(8X,E12.5))
C    WRITE(2,2010)(J,OCOAL(I),COAL(I),STREAM1(I),STREAM2(I),I=35,38)
     WRITE(2,2012)PCPSREM,OCOAL(39),COAL(39),STREAM1(39),STREAM2(39),
    -BTUREM,OCOAL(40),COAL(40),STREAM1(40),STREAM2(40),
    -BTUREM,OCOAL(41),COAL(41),STREAM1(41),STREAM2(41)
2012 FORMAT(1X,*PYRITIC SULFUR*,T20,E12.5,4(8X,E12.5)/
    -1X,*CARBON*,T20,E12.5,4(8X,E12.5)/
    -1X,*BTU*,T20,E12.5,4(8X,E12.5))
C    WRITE(2,2010)(J,OCOAL(I),COAL(I),STREAM1(I),STREAM2(I),I=42,50)
     RETURN
     END
```

```
TOTAL  INPUT  COAL:     .10000E+06
          FRACTION  COAL  REMOVAL:    .1918            TOTAL  CLEAN  COAL     .87340E+05
CONSTITUENT           FRACTION  REMOVED     INPUT  COAL              CLEAN  COAL       STREAM1          STREAM2
-----------           ----------------      ----------               ----------        -------          -------

ASH                      .58190E+00           .18700E+05               .11518E+05        .70022E+04       .17954E+03
TOTAL  SULFUR            .10600E+00           .30000E+04               .23884E+04        .59631E+03       .15290E+02
ANTIMONY                 .15000E+00           .70000E-01               .63070E-01        .67567E-02       .17325E-03
ARSENIC                  .58190E+00           .27000E+01               .16631E+01        .10110E+01       .25924E-01
BERYLLIUM                .20278E+00           .50000E+00               .43308E+00        .65244E-01       .16729E-02
CADMIUM                  .26806E+00           .12500E+00               .10288E+00        .21562E-01       .55288E-03
CHROMIUM                 .36072E+00           .30000E+01               .22858E+01        .69637E+00       .17856E-01
COPPER                   .38899E+00           .11800E+01               .87706E+00        .29537E+00       .75736E-02
IRON                     .43149E+00           .27000E+04               .19311E+04        .74969E+03       .19223E+02
LEAD                     .58190E+00           .11400E+01               .70218E+00        .42687E+00       .10946E-01
MAGNESIUM                .30000E+00           .11800E+03               .94636E+02        .22780E+02       .58410E+00
MANGANESE                .43149E+00           .74000E+01               .52926E+01        .20547E+01       .52685E-01
MERCURY                  .58190E+00           .17000E-01               .10471E-01        .63657E-02       .16322E-03
NICKEL                   .35264E+00           .20000E+01               .15345E+01        .45385E+00       .11637E-01
SELENIUM                 .37033E+00           .20000E-01               .15112E-01        .47662E-02       .12221E-03
SILVER                   .27601E+00           .10000E-01               .81783E-02        .17761E-02       .45542E-04
THALLIUM              0.                      .10000E+01               .10000E+01     0.               0.
ZINC                     .43149E+00           .16900E+01               .12087E+01        .46925E+00       .12032E-01
URANIUM                  .20995E+00           .70000E-01               .60300E-01        .94572E-02       .24249E-03
THORIUM                  .20995E+00           .66000E+00               .56855E+00        .89168E-01       .22864E-02
RADIUM-226               .58190E+00           .23660E-07               .14573E-07        .88595E-08       .22717E-09
RADIUM-228               .58190E+00           .26466E-09               .16302E-09        .99102E-10       .25411E-11
LEAD-210                 .58190E+00           .30590E-09               .18842E-09        .11454E-09       .29370E-11
HYDROCARBONS                                0.                       0.                0.               0.
TOTAL  SOLID  WASTE      .19181E+00         0.                       0.                  .12398E+05       .34999E+03
WATER                                       0.                       0.                  .10237E+04       .58331E+02
PYRITIC  SULFUR          .43149E+00           .18700E+04               .13375E+04        .51923E+03       .13314E+02
CARBON                   .10600E+00           .64100E+05               .59616E+05        .43723E+04       .11211E+03
BTU                      .10600E+00           .23000E+13               .21391E+13     0.               0.
```

2 SOLID WASTE MODULE FOR COAL COMBUSTION IN A CONVENTIONAL BOILER

2.1 Introduction

The largest volume of solid waste from energy industries currently and expected in the near future comes from conventional coal combustion. Increasingly stringent air regulations will require all new coal-fired power plants to employ flue gas desulfurization (FGD) processes to remove SO_2, and this will greatly increase the quantities of waste produced.

2.2 General Description of Solid Waste from Coal Combustion

Two types of ash are produced during combustion, fly ash consisting of the fine particles that are entrained in the flue gas stream, and bottom ash which is the coarser, heavier residue accumulated at the furnace bottom. The distribution of ash between bottom ash and fly ash fraction is a function of boiler type (firing method). Stoker fuel units emit the smallest proportion of fly ash, ~10%. In cyclone units, ~60% appears as fly ash; for other pulverized boilers (most commonly used by utilities) the split is 80% fly ash and 20% bottom ash.

In all cases utility and industrial boilers employ some form of precipitator to collect a proportion of the fly ash. The efficiency of the collection device and hence the amount of fly ash solid waste is highly variable. Depending on air regulations governing a particular facility, an FGD system may be needed.

The removal of SO_2 by means of scrubbers is accomplished by two general processes - throwaway and regenerable. The first type refers to those flue gas desulfurization scrubbers that produce a solid waste stream not presently marketable and requiring disposal. The most common example is a lime/limestone scrubber which uses calcium salts to absorb SO_2 in solution.

Regenerable scrubber systems are those which, because of their specific chemical reactions, produce a marketable product of sulfur and regenerate the sorbent which can be reused. Some common examples of regenerable processes are the Wellman-Lord sulfite and the magnesium oxide processes, both of which produce a usable sulfur product, such as solid elemental sulfur, liquid sulfuric acid, or highly concentrated SO_2 gas.

The throwaway systems may be either wet or dry. The wet scrubbing systems employ a slurry of either lime or limestone to remove the SO_2 and produce a waste consisting of calcium sulfate, calcium sulfite, and unreacted limestone. The major dry systems are a spray drier or dry injection. In the spray drier, the flue gas is contacted with a calcium-based slurry or sodium solution such that the gas is evaporated to apparent dryness. The dry injection system involves the introduction of a dry sorbent, the most promising being nahcolite (sodium bicarbonate), into the flue gas. The resulting waste, consisting of a dry mixture of sodium or calcium sulfite and sulfate, is collected by a baghouse precipitator. A major difference between the dry and wet systems is that in the majority of wet systems, the ash is collected by a precipitator prior to the scrubber, whereas in the dry systems the ash and scrubbing waste are collected together.

The wet throwaway processes are at present preferred by the utilities for several reasons including lower capital costs, availability and ease of use of sorbent and relative simplicity. But they have the major disadvantage of producing large amounts of waste. No dry systems are operating now commercially. The dry systems do not at present achieve as high a degree of SO_2 removal as do the wet systems.

2.3 Overall Module Description

The module computes the air and solid waste residuals which result from the combustion of coal in a conventional utility or industrial boiler. The input to the module is the quantity of coal and its composition in terms of sulfur, ash, and trace element content. The module employs a mass balance approach to compute the distribution of the sulfur, ash, and trace elements in the coal between the air and solid waste residuals. Figure 2.1 gives an overall view of the module.

The module calculates the air and solid waste residuals for four types of boiler:

General pulverized utility and large industrial boiler (>100m Btu/hr)
Cyclone utility and large industrial boiler (>100m Btu/hr)
Large industrial pulverized boiler (10 to 100m Btu/hr)
Small industrial stoker boiler (<10m Btu/hr)

An input variable determines which boiler is to be used.

A choice is then made as to the control mechanisms to be employed. A switch is set to determine whether the plant uses a precipitator to collect particulates either alone or followed by a FGD system to remove SO_2, or the plant employs only a FGD system to remove both SO_2 and particulates. At present the module considers only one generic type of precipitator, as there are not enough data available to assess what effect different systems (e.g., electrostatic precipitator or baghouse) have on trace element removal. The module could easily be expanded to include different devices. Both

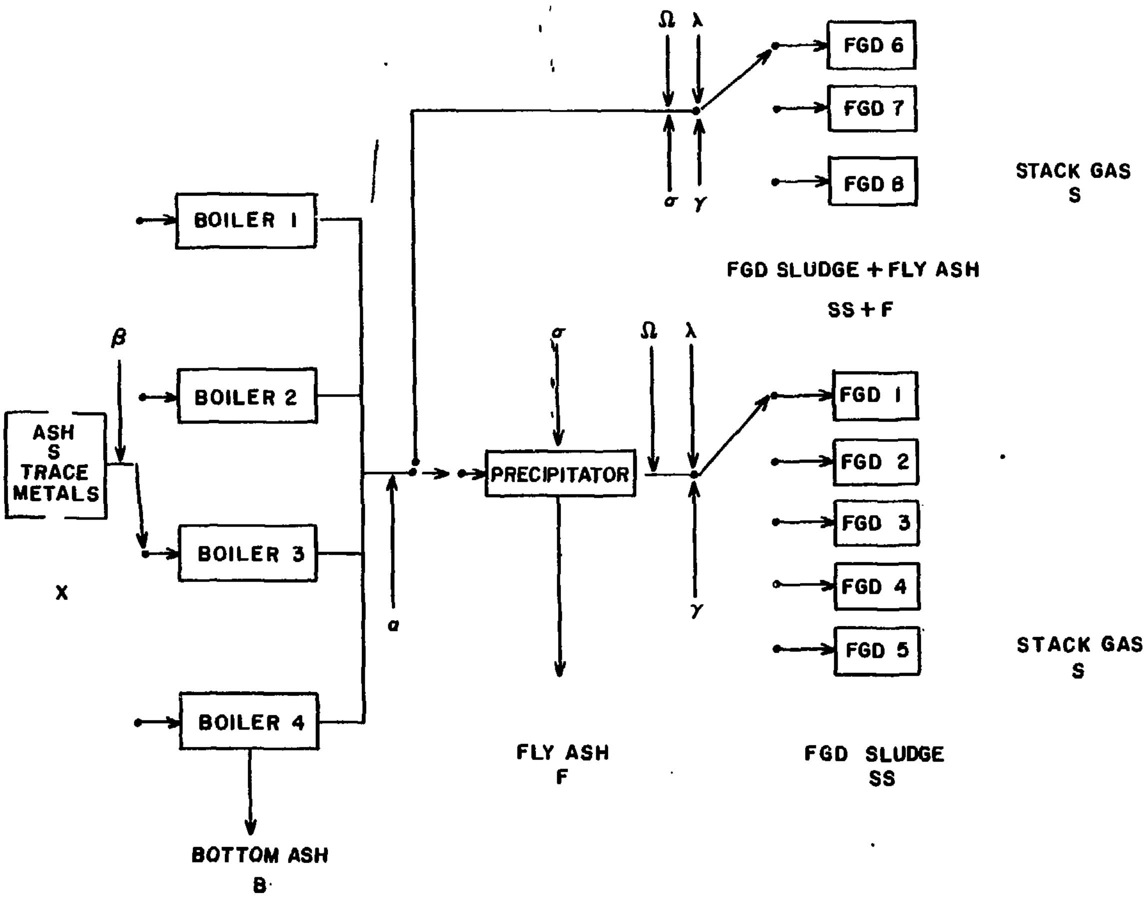

Figure 2.1. Overall conventional combustion module design.

Notation for Figure 2.1

Inputs

χ	Coal characteristics
β	Boiler type
α	Removal equipment used
	a. Precipitator followed by an FGD system
	b. FGD system only
σ	Percentage removal of TSP
Ω	Percentage removal of SO_2
λ	Type of FGD system
γ	Trace metal content of the scrubbing media

Outputs

B	Amount and composition of bottom ash
F	Amount and composition of fly ash
SS	Amount and composition of FGD sludge
S	Composition of stack gases

particulate and trace metal removals are given as a function of the efficiency of the precipitator. Any reasonable precipitator efficiency can be used; this is specified as an input variable.

The module uses 3 wet and 1 dry nonregenerable systems and 2 regenerable processes. The dry system used is injection of nahcolite into the flue gas followed by baghouse collection. The particulates are also removed in the baghouse.

Nonregenerable Systems:	Regenerable Systems:
Lime wet scrubbing.	Wellman-Lord sulfite scrubbing.
Limestone wet scrubbing.	Magnesia slurry absorption.
Double alkali wet scrubbing.	
Dry sorbent injection.	

If, however, a wet FGD system is to be used to remove both SO_2 and particulates, only a wet lime or limestone scrubber is considered. The dry FGD system also removes SO_2 and particulates. A switch is also set to determine the type of FGD system to be employed:

1. Precipitator followed by lime scrubber.
2. Precipitator followed by limestone scrubber.
3. Precipitator followed by double-alkali.
4. Precipitator followed by magnesium-oxide.
5. Precipitator followed by Wellman-Lord.
6. Lime scrubber only.
7. Limestone scrubber only.
8. Dry sorbent injection.
9. Precipitator only. No FGD system.

The module is called as a subroutine with the following arguments:

Input vector of coal characteristics.

Output vector of bottom ash composition.

Output vector of fly ash composition.

Output vector of FGD sludge composition.

Output vector of stack gas composition.

Type of boiler. Input integer number from
  1 to 4 corresponding to the type of boilers
  given on page 57.

Is a precipitator used or not? Input integer
  number, 1 or 0 respectively.

Type of FGD system. Input integer number from
  1 to 9 corresponding to the types shown on page 60.
  Input real number giving percentage removal of SO_2.
  Input real number giving percentage removal of
  particulates.
  Input quantity of coal.

To facilitate computation, the first 5 arguments are vectors which contain the same number of elements. These elements are given in Table 2.1. In all cases the elements are given as quantitites. Depending on which vector is being considered, a number of the elements will have zero values.

For radionuclides, data are, at present, only generally available for the input quantities of uranium and thorium. However, the masses of radium-226 and lead-210 can be calculated from the mass of uranium-238 and the mass of radium-228 from thorium-232. The equations and assumptions used in the calculation are given in Section 7.

Table 2.1
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda-ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

2.4 Description of Boiler Residuals

Depending on the type of boiler used, the elements of the input coal characteristics vector are multiplied by different sets of coefficients to give the quantity of each element which goes up the stack in the flue gas or fly ash. Table 2.2 gives the coefficients used. The coefficients are contained in external data files, and the values can therefore be easily changed as better data become available.

The figures for ash and sulfur are taken from Reference 1, with the exception of the coefficient for ash for cyclone utility boilers, which comes from References 2 to 5. The figure for carbon is taken from Reference 14. A number of reports were studied to obtain coefficients for the trace elements.[2-7] Reference 2 gives the results of trace metal distribution for two pulverized and one cyclone utility boilers. References 3 to 5 are all part of the same project undertaken by Oak Ridge National Laboratory to study the fate of trace elements at the Allen Plant which has a cyclone boiler. Figures from Reference 5 were used as this gives two sets of results for runs undertaken in 1972 and 1973. Reference 6 looked at trace element distribution at the Widows Creek Plant which has a pulverized boiler. Unfortunately, the report contains some rather spurious results for the split between bottom and fly ash, probably because there is a superheater, after the main boiler and before the precipitator, from which ash is collected. It was therefore decided not to include the results in the calculation of the coefficients. Reference 7 was a study of the Valmont Power Plant which uses a pulverized boiler. Again, the results could not be used in the calculation of the coefficients, because complete sets of results were available for only five of the trace elements and, of these, two had very poor mass balances.

Table 2.2
Boiler Coefficients for Fraction of the Incoming Element which Goes Up the Stack

Input Element	Boiler 1 Pulverized >100m Btu/hr	Boiler 2 Cyclone >100m Btu/hr	Boiler 3 Pulverized 10-100m Btu/hr	Boiler 4 Stoker <10m Btu/hr
Ash	0.80	0.40	0.65	0.10
Sulfur	0.95	0.95	0.95	0.95
Antimony	0.9483	0.9166	0.9483	0.9166
Arsenic	0.98	0.8271	0.98	0.8271
Beryllium	0.8371	0.418	0.8371	0.418
Cadmium	0.8818	0.8144	0.8818	0.8144
Chromium	0.878	0.5415	0.878	0.5415
Copper	0.8745	0.6892	0.8745	0.6892
Iron	0.7614	0.3946	0.7614	0.3946
Lead	0.9435	0.9256	0.9435	0.9256
Magnesium	0.8255	0.3786	0.8255	0.3786
Manganese	0.8466	0.3722	0.8466	0.3722
Mercury	0.9872	0.9877	0.9872	0.9877
Nickel	0.8422	0.7377	0.8422	0.7377
Selenium	0.9882	0.8066	0.9882	0.8066
Silver	0.9449	0.78	0.9449	0.078
Thallium	0.8807	0.9739	0.8807	0.9739
Zinc	0.8863	0.9288	0.8863	0.9288
Uranium-238	0.6997	0.5424	0.6997	0.5424
Thorium-232	0.8019	0.3874	0.8019	0.3874
Radium-226	0.80	0.40	0.65	0.10
Radium-228	0.80	0.40	0.65	0.10
Lead-210	0.9435	0.9256	0.9435	0.9256
Carbon	0.98	0.98	0.98	0.98

The coefficients for pulverized boilers were calculated from two sets of figures given in Reference 2. In all the studies, there was variability between elements as to how good the total mass balances were. In general, considering the experimental difficulties that must have arisen, the results are not too bad and in many cases the overall mass balances were reasonably close to unity. In order to calculate coefficients, the percentage splits between bottom and fly ash were normalized to give an overall mass balance of 100%. A geometric mean was then taken of the two sets of figures to give overall coefficients to calculate the fraction of the incoming element which goes up the stack in a pulverized boiler.

For the cyclone boiler, the two sets of results in Reference 5 and the figures for the cyclone boiler in Reference 2 were used. Again, the figures were normalized to give a mass balance of 100% and geometric means were taken.

Full details of the figures and calculations used are given in Appendix 2A. The figures clearly contained some analytical errors. Also, for some elements there were large variations in the results obtained by different teams and, in the case of the Oak Ridge Project, between different years. To produce good coefficients, additional experimental work is needed and as data become available the figures should be reviewed.

For Pb^{210} the same coefficients are used as for the nonradioactive isotope. Reference 12 indicated that for radium there is no significant enrichment or depletion in the bottom ash. It was therefore assumed that the split is the same as for the overall ash.

In particular, there were no available data on the trace metal distributions for medium and small industrial boilers. It was assumed that, based on the bottom to fly ash split, the medium-sized industrial boiler behaved more like the large pulverized boiler and the small industrial boiler like the cyclone boiler. The relevant sets of coefficients for trace elements were therefore used.

This is clearly unsatisfactory and the coefficients should be recalculated as soon as data become available.

The quantity of each element in the bottom ash is calculated by subtracting the quantity going up the stack from the original input quantity. This gives the output vector for bottom ash. The element named ash in this case refers to the total quantity of dry bottom ash.

After the amounts of sulfur and carbon in the bottom ash have been calculated, the remaining sulfur in the stack gas is converted to SO_2 by multiplying by 2 and the carbon to CO_2 by multiplying by 3.67. The output quantities then appear under element 35, sulfur dioxide, and element 42, carbon dioxide. Elements 35 to 37 are the gaseous pollutants, NO_2, CO, and CH_4, which are formed in the combustion process and appear in the final stack gas. They are calculated by multiplying the quantity of input coal by a set of coefficients, which again depend on the boiler type. The coefficients come from Reference 1 and are given in Table 2.3. This procedure does lead to a double counting of the carbon, but the fraction appearing as CO and CH_4 is very small compared to the CO_2.

2.5. Description of Precipitator Residuals

The composition of the stack gas from the boiler is used as an input to the precipitator. The efficiency of the precipitator, as a percentage, is given as an input variable.

Table 2.3
Coefficients for Calculation of Air Emissions

Pollutant	Emission Coefficients (tons/ton input coal) Boiler 1 Pulverized >100m Btu/hr	Boiler 2 Cyclone >100m Btu/hr	Boiler 3 Pulverized 10-100m Btu/hr	Boiler 4 Stoker <10m Btu/hr
NO_2	9.0×10^{-3}	2.75×10^{-2}	7.5×10^{-3}	3.0×10^{-3}
CO	5.0×10^{-4}	5.0×10^{-4}	1.0×10^{-3}	5.0×10^{-3}
CH_4	1.5×10^{-4}	1.5×10^{-4}	5.0×10^{-4}	1.5×10^{-3}

In other studies, the emission coefficients for trace metals have been calculated as being independent of the precipitator efficiency, which is clearly incorrect. In this module, attempts have been made to determine the quantity of each trace element passing through a precipitator as a function of the precipitator efficiency.

The measurements given in Reference 5 and stations II and III from Reference 2 were from boilers fitted with precipitators of differing efficiencies. For all results the percentage of the element passing through the precipitator was calculated. These figures could then be compared with the general pass-through of the fly ash. Table 2A.12, Appendix 2A, gives the results. In some cases the pass-through varied in a linear fashion with the increasing precipitator efficiency (e.g., iron and magnesium). In other cases a nonlinear function was found to better fit the points (e.g., arsenic, thorium). Table 2.4 gives the coefficients.

In some cases the coefficients are thought to be reasonably good (e.g., iron and manganese). However, for others the data were either not available or appeared spurious which leads to a low degree of confidence in the coefficient (e.g., lead, arsenic, and selenium). A full discussion of the

Table 2.4
Coefficients to Calculate the Function of a Trace Element
Passing Through a Precipitator

Element	Coefficient
Ash	P_{TP}
Antimony	$25.84\ \mathrm{Ln}(P_{TP} + 1)$
Arsenic	$6.84\ \mathrm{Ln}(P_{TP} + 1)$
Beryllium	P_{TP}
Cadmium	$15.23\ \mathrm{Ln}(P_{TP} + 1)$
Chromium	$2.05\ P_{TP}$
Copper	$1.25\ P_{TP}$
Iron	P_{TP}
Lead	$19.19\ \mathrm{Ln}(P_{TP} + 1)$
Magnesium	P_{TP}
Manganese	P_{TP}
Mercury	0.975
Nickel	$2.33\ P_{TP}$
Selenium	$20.84\ \mathrm{Ln}(P_{TP} + 1)$
Silver	$0.58\ P_{TP}$
Thallium	$2.69\ P_{TP}$
Zinc	$1.73\ P_{TP}$
Uranium - 238	$1.97\ P_{TP}$
Thorium - 232	$0.86\sqrt{P_{TP}}$
Radium - 226	$1.5\ P_{TP}$
Radium - 228	$1.5\ P_{TP}$
Lead - 210	$19.19\ \mathrm{Ln}\ (P_{TP} + 1)$

P_{TP} = Precipitator pass through = 100 - precipitator efficiency.

calculations and assumptions behind the coefficients is given in Appendix 2A together with a discussion of the degree of confidence in the accuracy of each coefficient. Clearly more data are required to enable the calculation of more reliable coefficients.

The quantity of each element in the fly ash is calculated by subtracting the quantity going out the stack after the precipitator from the input quantity into the precipitator. This gives the output vector for fly ash. The element named ash in this case refers to the total quantity of dry fly ash.

2.6 Description of FGD Residuals When the FGD Follows a Precipitator

The composition of the stack gas from the precipitator is used as an input to the FGD system. The switch determining which particular type of FGD system and its efficiency in terms of SO_2 removal are given as input variables.

Major Components. Although most of the particulates will have been removed prior to the FGD system, a small percentage will go into and be captured by the FGD unit. The total quantity of solid waste produced (element 25) is therefore the total quantity of FGD sludge plus the captured fly ash. This is given as the wet quantity. The individual components which make up total solid waste, element 1 (ash) and elements 26 to 33 (FGD sludge compounds) are given as dry weights. Element 34 (water) is the total amount of water (in tons) that is included in the total wet solid waste. The quantities of FGD scrubber sludge vary even within the same type of FGD process because of differences in working conditions. The equations used include variables which reflect these differences. At present, however, there are not many data available and default values have been substituted which reduces the equation to simple coefficients. The equations and assumptions used are given in Appendix 2B, and Table 2.5 sets out the coefficients used in the module.

Not many data were available to determine how much of the fly ash would be captured by the FGD system. From Reference 9 (pp. 4-45), figures were obtained which gave the percentage pass-through of fly ash as a function of input concentration. This showed that the pass-through varied from 45% at very low input concentrations to 5% at very high input concentrations.

Table 2.5
Coefficients to Calculate FGD Sludge and Its Major Components for Wet Scrubbing Systems

Component	Coefficient FGD1 Lime	FGD2 Limestone	FGD3 Double-Alkali	FGD4 Magnesium-Oxide	FGD5 Wellman-Lord
Total FGD sludge (wet)	4.728 SO_2	4.697 SO_2	4.6518 SO_2	0.1539 SO_2	0.2158 SO_2
Unreacted limestone (dry)	0.174 SO_2	0.3525 SO_2	0.0829 SO_2	N/A	N/A
Calcium sulfate (dry)	0.674 SO_2	0.631 SO_2	0.675 SO_2	N/A	N/A
Calcium sulfite (dry)	1.516 SO_2	1.365 SO_2	1.518 SO_2	N/A	N/A
Magnesium oxide (dry)	N/A	N/A	N/A	0.01875 SO_2	N/A
Magnesium sulfite (dry)	N/A	N/A	N/A	0.08125 SO_2	N/A
Soda ash (dry)	N/A	N/A	0.05 SO_2	N/A	N/A
Sodium bisulfite (dry)	N/A	N/A	N/A	N/A	0.08125 SO_2
Sodium sulfite (dry)	N/A	N/A	N/A	N/A	0.059 SO_2

N/A Not applicable.
SO_2 Quantity of captured SO_2.

A plant having a precipitator followed by an FGD system will be of recent construction and therefore will be subject to high particulate controls. This will give a low concentration of fly ash into the FGD system. It was therefore decided that until better data become available, 65% of the incoming fly ash would be captured by the FGD system.

Outlet fly ash (dry) = Inlet fly ash · 0.65.

This figure appears in the output vector as element 1 (ash). In the total solid waste (element 25), the quantity of wet fly ash is used.

$$\text{Fly Ash (wet)} = \text{Fly Ash (dry)} \times \frac{100}{100 - m},$$

where

m = moisture content.

The value of m will be the same as for the FGD sludge:

m = 50% for nonregenerable systems.

m = 35% for regenerable systems.

Total solid waste = FGD sludge + fly ash (wet).

Minor Components. Trace elements in the solid waste come from both the incoming combustion flue gas and the scrubbing media.

Trace Elements from Scrubbing Media. Table 2.6 gives the average trace metal content of lime and limestone (weight fraction). These figures are geometric averages of values given in References 8 and 10.

Table 2.6
Fraction of Trace Elements in Lime and Limestone

Trace Element	Lime	Limestone
Antimony	N/D	N/D
Arsenic	1.5×10^{-6}	1.71×10^{-6}
Beryllium	1.8×10^{-9}	1.87×10^{-7}
Cadmium	3.372×10^{-8}	1.55×10^{-7}
Chromium	3.12×10^{-6}	8.14×10^{-6}
Copper	1.9×10^{-6}	1.69×10^{-6}
Iron	6.27×10^{-8}	6.27×10^{-8}
Lead	2.07×10^{-7}	1.29×10^{-6}
Magnesium	7.68×10^{-3}	7.68×10^{-3}
Manganese	1.55×10^{-4}	1.55×10^{-4}
Mercury	N/D	N/D
Nickel	N/D	N/D
Selenium	1.74×10^{-5}	8.27×10^{-7}
Silver	N/D	N/D
Thallium	N/D	N/D
Zinc	1.96×10^{-4}	1.08×10^{-4}
Uranium	N/D	N/D
Thorium	N/D	N/D
Radium-226	N/D	N/D
Radium-228	N/D	N/D
Lead-210	N/D	N/D

N/D No results available.

No data were found for the trace metal content of the scrubbing media used in the regenerable processes. Since very little of the media ends up as solid waste, no account has been taken of its trace elements.

The total quantity of lime or limestone required depends on the amount of SO_2 to be removed. The equations and default values used to compute the amount of scrubbing media are given in Appendix 2B. The resulting coefficients are as follows:

Lime. Quantity of lime = 0.975 SO_2 tons.

Limestone. Quantity of limestone = 1.7625 SO_2.

Double Alkali. Quantity of lime = 0.925 SO_2.

In the above,

SO_2 = quantity of SO_2 captured.

The quantity of scrubbing media is multiplied by the coefficients in Table 2.6 to give the trace metals in the FGD sludge.

Trace Elements from Combustion Flue Gas. No reports were available which gave any data on the fate of trace elements in a plant where there is a high efficiency precipitator followed by a FGD system. Until data become available it is assumed that for all elements, except mercury, the pass-through is the same as for fly ash (35%). In fact there will be very little of each element entering the FGD system as most of it will have been removed in the fly ash. For mercury, a figure of 87% pass-through is used. This is the figure given in Reference 2 for a plant fitted with an FGD system to remove both particulates and SO_2. Since such a small fraction of the mercury is removed by a precipitator, its presence before a FGD system will probably have very little effect on the removal of mercury by the FGD system.

For the regenerable systems, only a small fraction of the scrubbing media appears as solid waste. The fate of the trace metals during the regeneration process is unknown at present. Most of the trace metals probably remain in the regenerated scrubbing media and a concentration will build up until an equilibrium is reached. However, there are no data available to say how much concentration there is. At present the module simply assumes that 8% of the scrubbing media appears as solid waste and therefore 8% of the incoming trace metals also come out in the solid waste. The quantities are in any case very small.

Total Trace Elements. The two sources of trace elements are added together. The output vector for FGD waste gives the total amount of dry trace elements.

2.7 Description of FGD Residuals for an FGD System Only

The composition of the stack gas from the boiler is used as an input to the FGD system. The switch determining which particular type of FGD system and its efficiency in terms of SO_2 removal are given as input variables. The use of a lime or a limestone wet scrubber or a dry sorbent injection system was assumed.

Major Components. In this case all the captured particulates appear with the FGD waste. The quantity of fly ash will depend on the efficiency of the system and is calculated as follows:

$$Q_{FA} = Q_{FAS} \cdot \sigma/100,$$

where

Q_{FAS} = quantity of fly ash entering FGD system.

σ = percentage removal of particulates (given as an input variable).

This gives the dry quantity of ash which is shown in the output under element 1 (ash). For wet FGD systems the total solid waste (element 25) is given as a wet quantity and includes the wet ash. Again the moisture content of the ash is assumed to be the same as for the overall FGD system. For dry sorbent injection, the total solid waste is a dry amount. There is no separate output vector to describe the fly ash.

For wet systems, the other major components are identical to those where the FGD system follows a precipitator.

Table 2.7 gives the coefficients used for the dry sorbent system. The equations and assumptions used are given in Appendix 2B. Since this system is not commercially operational, there are very few data on the variables such as the stoichiometric ratio of SO_2 to sorbent required to achieve a certain level of SO_2 removal and the sorbent utilization. The coefficients should therefore be treated as tentative and should be updated as more data become available.

Minor Components. For wet systems the calculation of the trace metals from the scrubbing media is identical to that for a FGD system following a precipitator. In the case of the trace metals from the flue gas, Reference 2 gives results for a plant where a FGD system is used to remove particulates and SO_2. The results are given in Appendix 2A, Table 2A.17. However, in this case the amount of trace elements passing through the FGD system will depend on the removal rate for particulates. Unfortunately, as results are available for only one plant, relationships between fly ash removal and trace metal removal cannot be established. Until more data become available it was decided to use the same coefficients as for the precipitator rather than to

Table 2.7
Coefficients To Calculate FGD Waste and Its Major Components for a Dry Sorbent Injection System

Component	Coefficient
Total FGD solid waste	3.075 SO_2
Sodium bicarbonate	0.046 SO_2
Sodium carbonate	0.781 SO_2
Sodium sulfate	1.605 SO_2
Sodium sulfite	0.643 SO_2

give only one removal rate regardless of fly ash capture, which would have occurred had the results from Reference 2 been used.

The only exception to this is mercury. From Reference 2 it would appear that a FGD system removes more mercury than a precipitator and both are probably independent of the fly ash removal rate. A figure of 87% pass-through is therefore assumed.

For the dry sorbent injection system there are no trace element data available. Again the same coefficients are used as for a precipitator, which is a reasonable assumption since the ash is being collected in a baghouse precipitator. The trace elements from the sorbent should be added to those in the ash; however, at present there are no data for the trace element content of nahcolite.

2.8. Description of Stack Gas Residuals

A final output vector gives the composition of the stack gas. For elements 1 and 3 to 23 this is the remainder of the input which has not been captured in the bottom ash, fly ash, or FGD sludge. Element 2 (sulfur) and element 40 (carbon) will be zero and element 30 will give the quantity of SO_2 not captured by the FGD system and element 42 the quantity of CO_2 formed.

Elements 36 to 38, NO_2, CO, and CH_4 are calculated from the coal input as boiler residuals and the amounts are passed through unaltered to appear in the stack gas output.

2.9. Computer Code

A description of the computer code used is given in Appendix 2C. In Appendix 2D there is a copy of the code along with a sample input and output.

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APPENDIX 2A

CALCULATION OF BOILER COEFFICIENTS

2A.1 Bottom Ash

Utility Pulverized Boiler. Coefficients were calculated from Reference 2, which gives results for two stations with pulverized boilers (station I and station II). In general, the mass balances obtained were fairly close to unity, the major discrepancies being

Mercury Station II

Nickel Station II

Cadmium Stations I and II

Lead Stations I and II

Thorium Station I and II

Thallium Station I and II

The results had already been normalized in the report to give mass balances of 100%. Tables 2A.1, 2A.2, and 2A.3 give the results. An average figure for the percentage of an incoming trace element which remains in the bottom ash was calculated by taking the geometric mean of the figures for the two stations. The results are given in Table 2A.4. In order to produce coefficients for the module, a fraction rather than a percentage was used, and since the coefficients are for the amount going into the stack gas, the coefficients are 1 minus the amount in the boiler ash fraction.

Utility Cyclone Boiler. Coefficients were calculated from References 2 and 5. Reference 5 gave two sets of results for experiments conducted in 1972 and 1973.

Table 2A.1
Fraction of Elements Entering with Coal Discharged in Bottom Ash or Sluice Ash for Sampled Stations, Reference 2

Element	Station I Bottom Ash (21.3%)	Station II Sluice Ash (22.2%)	Station III Bottom Ash (63.1%)
Antimony	9.9	2.7	15.9
Arsenic	5.0	0.8	16.9
Beryllium	15.7	16.9	58.2
Cadmium	8.9	<15.7	26.8
Chromium	10.7	13.9	44.2
Copper	12.4	12.7	34.1
Iron	20.4	27.9	61.8
Lead	3.1	10.3	<7.8
Magnesium	17.7	17.2	62.1
Manganese	13.5	17.3	62.5
Mercury	0.78	2.1	<0.8
Nickel	18.3	13.6	22.7
Selenium	0.0	1.4	2.3
Silver	9.5	3.2	22.0
Thallium	11.5	12.33	2.6
Thorium	14.3	27.5	72.2
Uranium	50.1	18.0	42.7
Zinc	4.4	29.4	13.3

Table 2A.2
Fraction of Elements Entering with Coal Discharged in Economizer Ash Plus Scrubber Slurry or Cyclone Ash or Precipitator Ash for Sampled Stations, Reference 2

Element	Station I Economizer Ash & Scrubber Slurry (78.5%)	Station II Precipitator Ash (77.1%)	Station III Economizer Ash & Cyclone Ash (24.0%)
Antimony	89.4	93.4	6.2
Arsenic	87.6	99.1	62.6
Beryllium	83.8	81.0	35.0
Cadmium	84.2	80.5	32.5
Chromium	79.4	73.7	15.4
Copper	87.0	86.5	37.2
Iron	80.0	71.3	20.7
Lead	94.9	82.2	27.7
Magnesium	81.1	82.0	23.1
Manganese	85.9	81.5	25.2
Mercury	12.5	0.0	3.1
Nickel	77.6	68.2	14.3
Selenium	97.8	60.9	32.4
Silver	86.1	95.5	62.2
Thallium	65.4	82.2	5.9
Thorium	85.6	72.4	26.3
Uranium	47.8	80.5	17.8
Zinc	93.0	68.0	34.2

Table 2A.3
Fraction of Elements Entering with Coal Discharged in Flue Gas for Sampled Stations, Reference 2

Element	Station I Flue Gas (0.3%)	Station II Flue Gas (0.7%)	Station III Flue Gas (12.9%)
Antimony	0.61	3.9	77.9
Arsenic	7.5	0.05	20.5
Beryllium	0.65	<2.0	6.5
Cadmium	7.0	<3.8	41.1
Chromium	9.9	12.4	40.3
Copper	0.66	0.8	28.9
Iron	0.63	0.8	17.5
Lead	1.9	7.5	64.6
Magnesium	1.2	0.8	14.8
Manganese	0.38	1.2	12.5
Mercury	86.8	97.9	96.1
Nickel	4.1	18.2	62.8
Selenium	2.2	27.7	65.4
Silver	4.7	1.3	<15.9
Thallium	23.0	5.5	91.5
Thorium	0.1	0.1	1.5
Uranium	2.0	1.5	29.5
Zinc	2.5	2.6	52.7

Table 2A.4
Calculation of Average Percentage of Trace Elements which Remain in the Bottom Ash in a Pulverized Utility Boiler

Trace Element	Station I Bottom Ash (%)	Station II Bottom Ash (%)	Geometric Mean Bottom Ash (%)
Antimony	9.9	2.7	5.17
Arsenic	5.0	0.8	2.0
Beryllium	15.7	16.9	16.29
Cadmium	8.9	<15.7	11.82
Chromium	10.7	13.9	12.20
Copper	12.4	12.7	12.55
Iron	20.4	27.9	23.86
Lead	3.1	10.3	5.65
Magnesium	17.7	17.2	17.45
Manganese	13.5	17.3	15.34
Mercury	0.78	2.1	1.28
Nickel	18.3	13.6	15.78
Selenium	0.0	1.4	1.18
Silver	9.5	3.2	5.51
Thallium	11.5	12.3	11.9
Thorium	14.3	27.5	19.8
Uranium	50.1	18.0	30.0
Zinc	4.4	29.4	11.37

Again, in most cases the mass balances were good, the exceptions being

Antimony
Arsenic
Chromium
Copper (1972)
Mercury

The figures were recalculated to give overall mass balances of 100%, assuming that any imbalance was evenly distributed between the three fractions. Tables 2A.5 and 2A.6 give the normalized figures.

Reference 2 gave one set of results (station III). These results gave very good mass balances, the only serious imbalance being for mercury and thallium. The results had been normalized in the report and Tables 2A.1, 2A.2, and 2A.3 show the results obtained. An average figure for the percentage of an incoming trace element which remains in the bottom ash was calculated by taking the geometric mean of the 3 sets of results. Table 2A.7 gives the figures obtained. Again the coefficients were calculated as 1 minus the boiler fraction.

2A.2 Fly Ash and Stack Gas.

The figures giving the split between bottom, fly, and stack ash were recalculated for all 5 sets of results to reflect the average bottom ash content. Using the average bottom ash content for the boilers the figures for stack and fly ash were recalculated keeping their original ratios to again give a mass balance of 100%. Tables 2A.8 to 2A.12 give the results of these calculations.

Table 2A.5
Distribution of Trace Elements for a Cyclone Boiler Normalized to Give a Mass Balance of 100%, Reference 5 (1972)

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	N/D	N/D	N/D
Arsenic	20.00	72.01	7.99
Beryllium	N/D	N/D	N/D
Cadmium	N/D	N/D	N/D
Chromium	59.22	39.10	1.68
Copper	62.50	36.29	1.21
Iron	70.15	28.91	0.94
Lead	6.98	90.70	2.32
Magnesium	67.63	29.95	2.42
Manganese	74.87	24.06	1.07
Mercury	N/D	N/D	N/D
Nickel	N/D	N/D	N/D
Selenium	41.02	33.34	25.64
Silver	N/D	N/D	N/D
Thallium	N/D	N/D	N/D
Zinc	3.62	93.97	2.41
Uranium	63.90	35.14	0.96
Thorium	68.88	30.61	0.51

N/D No data available.

Table 2A.6
Distribution of Trace Elements for a Cyclone Boiler Normalized to Give a Mass Balance of 100%, Reference 5 (1973)

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	4.38	78.08	17.54
Arsenic	15.30	82.66	2.04
Beryllium	N/D	N/D	N/D
Cadmium	12.85	84.29	2.86
Chromium	36.83	62.32	0.85
Copper	14.08	85.34	0.58
Iron	51.19	48.49	0.32
Lead	7.57	89.40	3.03
Magnesium	57.14	42.86	0.00
Manganese	52.87	46.71	0.42
Mercury	1.89	3.77	94.34
Nickel	30.31	69.30	0.39
Selenium	76.68	22.36	0.96
Silver	N/D	N/D	N/D
Thallium	N/D	N/D	N/D
Zinc	7.50	90.83	1.67
Uranium	35.89	63.25	0.86
Thorium	46.26	53.58	0.36

N/D No data available.

Table 2A.7
Calculation of Average Percentage of Trace Elements which Remain in the Bottom Ash in a Cyclone Utility Boiler

Trace Element	Reference 2 Station III Bottom Ash (%)	Reference 5 1972 Bottom Ash (%)	Reference 5 1973 Bottom Ash (%)	Geometric Mean Bottom Ash (%)
Antimony	15.9	N/D	4.38	8.345
Arsenic	16.9	20.00	15.30	17.29
Beryllium	58.2	N/D	N/D	58.2
Cadmium	26.8	N/D	12.85	18.56
Chromium	44.2	59.22	36.83	45.85
Copper	34.1	62.50	14.08	31.08
Iron	61.8	70.15	51.19	60.54
Lead	<7.8	6.98	7.57	7.44
Magnesium	62.1	67.63	57.14	62.14
Manganese	62.5	74.87	52.87	62.78
Mercury	<0.8	N/D	1.89	1.23
Nickel	22.7	N/D	30.31	26.23
Selenium	2.3	41.02	76.68	19.34
Silver	22.0	N/D	N/D	22.0
Thallium	2.61	N/D	N/D	2.61
Zinc	13.3	3.62	7.50	7.12
Uranium	42.69	63.90	35.14	45.76
Thorium	72.17	68.88	46.26	61.26

N/D No data available.

2A.2.1 Coefficients for a Boiler Fitted With a Precipitator. The data from Reference 2, stations II and III, and Reference 5 are for boilers fitted with a precipitator for fly ash collection. The amount of most trace elements trapped in a precipitator will in some way depend on the precipitator efficiency. All four results came from plants using precipitators of differing efficiencies. The percentage of the total amount of each trace metal which passed through the precipitator into the stack gas was calculated. These figures could then be compared with the percentage pass-through of the fly ash, which are:

Reference 2	Station II	0.9%
Reference 2	Station III	35.0%

Table 2A.8
Distribution of Trace Elements, Pulverized Boiler, Station I, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	5.17	94.185	0.645
Arsenic	2.00	90.27	7.73
Beryllium	16.29	83.07	0.64
Cadmium	11.82	81.41	6.77
Chromium	12.20	78.06	9.74
Copper	12.55	86.79	0.66
Iron	23.86	75.55	0.59
Lead	5.65	92.50	1.85
Magnesium	17.45	81.34	1.21
Manganese	15.34	84.29	0.37
Mercury	1.28	12.43	86.29
Nickel	15.78	79.99	4.23
Selenium	1.18	96.65	2.17
Silver	5.51	89.60	4.89
Thallium	11.93	65.15	22.92
Zinc	11.37	86.31	2.32
Uranium	30.03	67.16	2.83
Thorium	19.81	86.62	0.08

N/D No data available.

Table 2A.9
Distribution of Trace Elements, Pulverized Boiler, Station II, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	5.17	91.03	3.80
Arsenic	2.00	97.95	0.05
Beryllium	16.29	81.69	2.02
Cadmium	11.82	84.20	3.98
Chromium	12.20	75.16	12.64
Copper	12.55	86.65	0.80
Iron	23.86	75.29	0.85
Lead	5.65	86.46	7.89
Magnesium	17.45	81.74	0.81
Manganese	15.34	83.43	1.23
Mercury	1.28	0.00	98.72
Nickel	15.78	66.48	17.74
Selenium	1.18	67.93	30.89
Silver	5.51	93.22	1.27
Thallium	11.93	82.56	5.51
Zinc	11.37	85.37	3.26
Uranium	30.03	68.69	1.28
Thorium	19.81	86.54	0.16

N/D No data available.

Table 2A.10

Distribution of Trace Elements, Pulverized Boiler, Station III, Reference 2, Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	8.345	6.755	84.90
Arsenic	17.29	62.31	20.40
Beryllium	58.20	35.0	6.5
Cadmium	18.56	35.96	45.48
Chromium	45.85	14.97	39.18
Copper	31.08	38.79	30.13
Iron	60.54	21.38	18.08
Lead	7.44	27.78	64.78
Magnesium	62.14	23.08	14.78
Manganese	62.78	24.88	12.34
Mercury	1.23	3.09	95.68
Nickel	26.23	13.68	60.09
Selenium	19.34	26.72	53.94
Silver	22.00	62.12	15.88
Thallium	2.61	5.94	91.46
Zinc	7.12	36.56	56.32
Uranium	45.76	16.81	37.43
Thorium	61.26	36.61	2.13

N/D No data available.

Table 2A.11

Distribution of Trace Elements, Reference 5 (1972), Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas.

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	N/D	N/D	N/D
Arsenic	17.29	74.45	8.26
Beryllium	N/D	N/D	N/D
Cadmium	N/D	N/D	N/D
Chromium	45.85	51.93	2.22
Copper	31.08	66.69	2.23
Iron	60.54	38.22	1.24
Lead	7.44	90.25	2.31
Magnesium	62.14	35.03	2.83
Manganese	62.78	35.63	1.59
Mercury	N/D	N/D	N/D
Nickel	N/D	N/D	N/D
Selenium	19.34	45.60	35.06
Silver	N/D	N/D	N/D
Thallium	N/D	N/D	N/D
Zinc	7.12	90.56	2.32
Uranium	45.76	52.80	1.44
Thorium	61.26	38.1	0.64

N/D No data available.

Table 2A.12
Distribution of Trace Elements, Reference 5 (1973), Using Average Boiler Fraction and Recalculating Fly Ash and Stack Gas

Trace Element	Bottom Ash (%)	Fly Ash (%)	Stack (%)
Antimony	8.345	74.845	16.81
Arsenic	17.29	80.72	1.99
Beryllium	N/D	N/D	N/D
Cadmium	18.56	78.77	2.67
Chromium	45.85	53.42	0.73
Copper	31.08	68.45	0.47
Iron	60.54	39.20	0.26
Lead	7.44	89.52	3.04
Magnesium	62.14	37.86	0.00
Manganese	62.78	36.89	0.33
Mercury	1.23	3.79	94.98
Nickel	26.23	73.36	0.41
Selenium	19.34	77.3	3.29
Silver	N/D	N/D	N/D
Thallium	N/D	N/D	N/D
Zinc	7.12	91.20	1.68
Uranium	45.76	53.51	0.73
Thorium	61.26	38.48	0.26

N/D No data available.

Reference 5	1972	3.5%
Reference 5	1973	0.5%

The results, given in Table 2A.13, were used in an attempt to derive a function for the percent pass-through (P_X) of each trace element (x) based on the percentage age pass-through (P_{TP}) of the fly ash, where

$$P_{TP} = 100 - (\text{efficiency of precipitator}).$$

Other research was also used to assist in deriving these functions. Two steps were used in arriving at these functions:

a) determination of functional relationship (i.e., linear, exponential, etc.),

b) calculation of a coefficient for that relationship.

Determination of Functional Relationships. Past studies[2,5] indicate that some trace metals are enriched after the flue gas passes through a precipitator and some are not, i.e., those that are enriched are in a higher proportion to the total mass output of the ash than they are to the total mass input to the precipitator.

The elements that are not enriched were assumed to be a linear function of P_{TP} with a coefficient of 1. Table 2A.14 shows the elements that are and are not enriched.

Trace elements that are enriched may be a linear or nonlinear function of P_{TP}. For these elements, the percent pass-through at the four power plants in Table 2A.13 were examined. For each element, the proportion

$$P_x(p_i)/P_x(p_j),$$

was calculated, where $P_x(p_i)$ = percentage pass-through of trace element x for a power plant with precipitator efficiency p_i, $i = 1,2,3,4$ and $p_i = .5, .9, 3.5, 35$. These proportions for the enriched trace elements are shown in Table 2A.15.

These results were then compared to proportions which would exist if P_x were various functions of P_{TP}, under the assumption that if

$$P_x(p_i) = C \cdot f(P_{TP}(p_i)),$$

where C is some coefficient, then

$$\frac{P_x(p_i)}{P_x(p_j)} = \frac{C \cdot f(P_{TP}(p_i))}{C \cdot f(P_{TP}(p_j))} = \frac{f(P_{TP}(p_i))}{f(P_{TP}(p_j))} .$$

The proportions for the various functions examined are in Table 2A.16.

When a trace element failed to resemble any theoretical function, possible spurious values were eliminated from Table 2A.13 and another comparison was made using only the remaining values.

Table 2A.13
Percentage Pass-Through of Trace Elements for Precipitators of Varying Efficiency

Trace Element	Reference 5 (1972) [0.5%][1]	Reference 2 Station II [0.9%][1]	Reference 5 (1973) [3.5%][1]	Reference 2 Station III [35%][1]
Antimony	18.34	4.01	N/D	92.63
Arsenic	2.41	0.05	9.99	24.66
Beryllium	N/D	2.41	N/D	15.66
Cadmium	3.28	4.51	N/D	55.84
Chromium	1.35	14.40	4.1	72.35
Copper	0.68	0.92	3.24	43.72
Iron	0.66	1.12	3.14	45.82
Lead	3.28	8.36	2.50	70.00
Magnesium	0.00	0.98	7.47	39.04
Manganese	0.88	1.45	4.27	33.17
Mercury	96.16	100.00	N/D	96.87
Nickel	0.55	21.1	N/D	81.45
Selenium	4.08	31.26	43.5	66.87
Silver	N/D	1.34	N/D	20.36
Thallium	N/D	6.25	N/D	93.9
Zinc	1.81	3.67	2.49	60.65
Uranium	1.34	1.83	2.65	69.0
Thorium	0.67	0.18	1.65	5.5
Radium	N/D	N/D	N/D	N/D

N/D No data available.

[1] Percentage pass-through for fly ash.

Table 2A.14
Enrichment of Trace Elements upon Passing through Precipitator

Enriched	Not Enriched
Antimony	Beryllium
Arsenic	Iron
Cadmium	Magnesium
Chromium	Manganese
Copper	
Lead	
Mercury	
Nickel	
Selenium	
Silver	
Thallium	
Zinc	

Table 2A.15
Ratios of Pass-Through of Trace Elements at Four Power Plants

Ratio	$\frac{P_x(.5)}{P_x(.9)}$	$\frac{P_x(.5)}{P_x(3.5)}$	$\frac{P_x(.5)}{P_x(35.)}$	$\frac{P_x(.9)}{P_x(3.5)}$	$\frac{P_x(.9)}{P_x(35.)}$	$\frac{P_x(3.5)}{P_x(35)}$.
Ratio ~	(1)	(2)	(3)	(4)	(5)	(6)
Antimony	4.57	N/D	0.198	N/D	0.043	N/D
Arsenic	48.2	0.241	0.098	0.005	0.002	0.405
Cadmium	0.727	N/D	0.059	N/D	0.081	N/D
Chromium	0.094	0.329	0.019	3.512	0.199	0.057
Copper	0.745	0.211	0.016	0.284	0.021	0.074
Lead	0.392	1.132	0.047	3.344	0.119	0.036
Mercury	0.962	N/D	0.993	N/D	1.032	N/D
Nickel	0.026	N/D	0.007	N/D	0.259	N/D
Selenium	0.131	0.094	0.061	0.719	0.467	0.651
Silver	N/D	N/D	N/D	N/D	0.066	N/D
Thallium	N/D	N/D	N/D	N/D	0.067	N/D
Zinc	0.493	0.727	0.030	0.180	0.061	0.041
Uranium	0.732	0.506	0.019	0.691	0.027	0.038
Thorium	3.72	0.406	0.122	0.109	0.033	0.300
Radium	N/D	N/D	N/D	N/D	N/D	N/D

N/D - No data available.

Table 2A.16
Theoretical Proportions of Trace Metal Pass-Through for Given Functions of Fly Ash Pass-Through

Function	f(.5)/ f(.9)	f(.5)/ f(3.5)	f(.5)/ f(35.)	f(.9)/ f(3.5)	f(.9)/ f(35)	f(3.5)/ f(35)
$f(P_{TP}) = 1$	1.0	1.0	1.0	1.0	1.0	1.0
$= P_{TP}$	0.556	0.143	0.014	0.257	0.026	0.100
$= P_{TP}^2$	0.309	0.020	0.0002	0.066	0.001	0.010
$= \sqrt{P_{TP}}$	0.745	0.378	0.120	0.507	0.160	0.316
$= \log(P_{TP} + 1)$	0.632	0.270	0.114	0.427	0.181	0.423
$= \sqrt{P_{TP} + 1}$	0.889	0.577	0.207	0.650	0.233	0.359
$= (P_{TP} + 1)^2$	0.623	0.111	0.002	0.178	0.003	0.016

If a trace element still failed to conform to a specific function, it was compared to elements with "known" functional relationships for similar characteristics (e.g., preferential adherence to various-sized particles in the flue gas[11]) and given the same function as those elements that were similar.

The determined function for each of the enriched elements is as follows:

Arsenic: Assuming that $P_{As}(.9) = 0.5$ is an analytic error, the proportions for As are similar to those for $f(P_{TP}) = \log(P_{TP} + 1)$, i.e., started log of P_{TP}.

Antimony, Cadmium, Selenium. These elements failed to conform to any function, but had similar particle-size adherence preferences to As (Reference 11). They were therefore assumed to be functions of the started log of P_{TP}.

Chromium, Nickel: These metals did not favorably compare to any one function of P_{TP}. However, they seemed concentrated evenly over different sized particles.[11] They were therefore assumed to be related to P_{TP} by a linear function.

Copper: Except for the proportion $P_{Cu}(.5)/P_{Cu}(.9)$, a linear trend is indicated.

Lead: Assuming that the value of $P_{Pb}(3.5)$ is an error, Pb seems more like a function of the started log of P_{TP}, although the proportions are highly variable.

Mercury: Proportions indicate almost 100% pass-through.

Silver: The proportion of Ag looks linear, and the actual values of the two silver measurements resemble those for Mn and Be. Although there are not many data, a linear relationship is assumed between P_{Ag} and P_{TP}.

Zinc: The value of $P_{Zn}(3.5)$ appears to be too small. All proportions not involving $P_{TP} = 3.5$ indicate a linear trend.

Thallium: There are only two data points for thallium. Their ratio falls between the linear and square root ratio. Since the ratio in Table 2A.15 looks similar to silver and zinc (which are linear in P_{TP}) the linear relation was chosen.

Radium: No data was available for radium. A linear relationship with coefficient 1.5 was chosen based on information in Reference 12.

Thorium: Thorium has a very low value for $P_{TP} = .9$. All ratios not involving this value indicate that thorium has a square root relation with P_{TP}.

Uranium: The uranium ratios are similar to either the linear or square root ratios. However, since the data are very similar to that of zinc, the linear relationship was chosen.

Calculation of Coefficients. After having decided upon the functional relations to be used, a coefficient was then calculated by doing a least squares regression on the values for each trace metal, using values which were not considered spurious, and forcing the line to go through the origin.

Table 2A.17 gives the coefficient, functional relationship, and comments for all trace elements which become enriched upon passing through the precipitator.

2A.2.2 Coefficients for a Boiler Fitted with a FGD System.

Reference 2, station I, gives results for a boiler followed by a scrubber for fly ash

Table 2A.17
Relation of Particulate Pass-Through to Enriched Trace Element Pass-Through for Enriched Trace Elements.

Trace Element	Coefficient	$f(P_{TP})$	Comments
Antimony	25.84	started log	used values at P_{TP} = .9,35
Arsenic	6.84	started log	used values at P_{TP} = .5,3.5,35
Cadmium	15.23	started log	used all available data points
Chromium	2.05	linear	used values at P_{TP} = .5,3.5,35
Copper	1.25	linear	used all values
Lead	19.19	started log	used values at P_{TP} = .5,.9,35
Mercury	.975	constant	assume constant pass-through 97.5%
Nickel	2.33	linear	used values at P_{TP} = .5,35
Selenium	20.84	started log	used all values
Silver	.58	linear	used all available data
Thallium	2.69	linear	used all available data
Zinc	1.73	linear	used values at P_{TP} = .5,.9,35
Uranium	1.97	linear	used all values
Thorium	0.86	square root	used values at P_{TP} 0.5,3.5,35
Radium-226	1.5	linear	assumed from Reference 12
Radium-228	1.5	linear	assumed from Reference 12
Lead-210	19.19	started log	assumed same as nonradioactive lead

collection. The figures taken from the results from plants fitted with precipitators were reworked to give the percentage of the total trace metal going into the FGD scrubber which passes through into the stack gas. This can be compared to the overall pass-through of the fly ash. Table 2A.18 gives the results. Unfortunately, since this was the only set of results, coefficients similar to those for passage through a precipitator could not be calculated.

Table 2A.18

Percentage Pass-Through of Trace Elements as Compared to the Pass-Through of Fly Ash for a Scrubber (Figures Taken from Reference 2, Station I

Trace Element	Reference 2, Station I (0.4%)[1]
Antimony	0.68
Arsenic	7.89
Beryllium	0.76
Cadmium	7.68
Chromium	11.10
Copper	0.75
Iron	0.77
Lead	1.96
Magnesium	1.46
Manganese	0.44
Mercury	87.4
Nickel	5.02
Selenium	2.20
Silver	5.17
Thallium	26.02
Zinc	2.62
Thorium	4.04
Uranium	0.09

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[1] Percentage pass-through for fly ash.

APPENDIX 2B

CALCULATION OF QUANTITY AND COMPOSITION OF FGD SLUDGE

2B.1 Equations Used To Calculate Quantity of FGD Sludge and Its Major *Components for Wet Scrubbing Systems.*

The equations were developed using a mass balance approach and the assumptions given in Reference 8. The default values are also taken from Reference 8. The equations are given below and the default values substituted into the equations are given in Table 2B.1. Table 2B.2 gives the chemical formulae and molecular weights used.

2B.1.1 Quantity of SO_2 Captured (tons)

$$SO_2 = SO_2FG \cdot \Omega/100,$$

where

SO_2FG = quantity of SO_2 entering FGD system,

Ω = percentage of removal of SO_2, given as an input variable.

2B.1.2 Lime Scrubber

Quantity of Lime Required (Q_{lime}) (tons)

$$Q_{lime} = SO_2\ (1 - U) + SO_2 \cdot \frac{MW\ lime}{MW\ SO_2},$$

$$Q_{lime} = 0.975\ SO_2.$$

where

SO_2 = quantity of SO_2 captured (tons),

U = absorbent utilization (fraction) molar basis,

MW = molecular weight

Table 2B.1
Default Values for Calculation of FGD Solid Waste

Variable	Lime	Limestone	Double-Alkali	Magnesium Oxide	Wellman-Lord
Absorbent utilization	90 %(36)	80 %(36)	95 %(36)	N/A	N/A
U	0.9	0.8	0.95	N/A	N/A
Sulfite: sulfate ratio	3.1(26)	3.1(26)	3.1(26)	N/A	N/A
X	3	3	3	N/A	N/A
Y	1	1	1	N/A	N/A
Soda-ash makeup	N/A	N/A	3 %(36)	N/A	N/A
SA	N/A	N/A	0.03	N/A	N/A
Moisture content (M)	50	50	50	35	35
Absorbent makeup	N/A	N/A	N/A	3 %(36)	3 %(36)
AB	N/A	N/A	N/A	0.03	0.03
Separation loss	N/A	N/A	N/A	5 %(36)	5 %(36)
SL	N/A	N/A	N/A	0.05	0.05

N/A Not applicable.
Figures in parenthesis refer to the appropriate page number in Reference 8.

Table 2B.2
Molecuar Weights of Compounds Used in FGD Systems

Compound	Chemical Formulae	Molecular Weight
Sulfur dioxide	SO_2	64
Lime	CaO	56
Limestone	$CaCO_3$	100
Calcium sulfite	$CaSO_3 \cdot 1/2H_2O$	129
Calcium sulfate (gypsum)	$CaSO_4 \cdot 2H_2O$	172
Sodium carbonate (soda-ash)	Na_2CO_3	106
Magnesium oxide	MgO	40
Magnesium sulfite	$MgSO_3$	104
Sodium sulfite	Na_2SO_3	126
Sodium bisulfite	$NaHSO_3$	104
Sodium bicarbonate	$NaCO_3$	84
Sodium carbonate	Na_2CO_3	106
Sodium sulfate	Na_2SO_4	142

<u>Sludge Solid Waste</u>. The sludge solids consist of: (1) unreacted lime in the form of limestone, (2) calcium sulfite [x parts], and (3) calcium sulfate [y parts].

Unreacted Limestone ($Q_{urlimestone}$) (tons)

$$Q_{urlimestone} = Q_{lime}\ (1 - U)\ .\ \frac{MW\ limestone}{MW\ lime}\quad .$$

$$Q_{urlimestone} = 0.174\ SO_2.$$

Calcium Sulfite ($Q_{calcium\ sulfite}$) (tons)

$$Q_{calcium\ sulfite} = Q_{lime} - (Q_{lime} \cdot (1 - U).\ \frac{x}{(x+y)}\ .\ \frac{MW\ calcium\ sulfite}{MW\ lime}$$

$$Q_{calcium\ sulfite} = 1.516\ SO_2.$$

Calcium Sulfate ($Q_{calcium\ sulfate}$) (tons)

$$Q_{calcium\ sulfate} = Q_{lime} - (Q_{lime} \cdot (1 - U).\ \frac{y}{(y+x)}\ .\ \frac{MW\ calcium\ sulfate}{MW\ lime}$$

$$Q_{calcium\ sulfate} = 0.674\ SO_2.$$

Total Sludge Solid Waste (Q_{TSW}) (tons)

$$Q_{TSW}(dry) = Q_{urlimestone} + Q_{calcium\ sulfite} + Q_{calcium\ sulfate}$$

$$Q_{TSW}(dry) = 2.364\ SO_2\ \text{tons}.$$

$$Q_{TSW}(wet) = Q_{TSW}(dry)\ .\ \frac{100}{(100-m)}\ ,$$

where

m = moisture content of FGD sludge,

$$Q_{TSW}(wet) = 4.728\ SO_2.$$

2B.1.3 Limestone Scrubber

Quantity of Limestone Required ($Q_{limestone}$) (tons)

$$Q_{limestone} = SO_2 \cdot (1 - U) + SO_2 \cdot \frac{MW\ limestone}{MW\ SO_2},$$

$$Q_{limestone} = 1.7625\ SO_2.$$

where

SO_2 = quantity of SO_2 captured,

U = absorbent utilization (fraction) molar basis.

Sludge Solid Waste. The sludge solids consist of: (1) unreacted limestone, (2) calcium sulfite [x parts], and (3) calcium sulfate [y parts].

Unreacted Limestone ($Q_{urlimestone}$) (tons)

$$Q_{urlimestone} = Q_{limestone} \cdot (1 - U),$$

$$Q_{urlimestone} = 0.3525\ SO_2.$$

Calcium Sulfite ($Q_{calcium\ sulfite}$) (tons)

$$Q_{calcium\ sulfite} = (Q_{limestone} - Q_{urlimestone}) \cdot \frac{x}{(x+y)} \cdot \frac{MW\ calcium\ sulfite}{MW\ limestone},$$

$$Q_{calcium\ sulfite} = 1.365\ SO_2$$

Calcium Sulfate ($Q_{calcium\ sulfate}$)(tons)

$$Q_{calcium\ sulfate} = (Q_{limestone} - Q_{urlimestone}) \cdot \frac{y}{(x+y)} \cdot \frac{MW\ calcium\ sulfate}{MW\ limestone},$$

$$Q_{calcium\ sulfate} = 0.631\ SO_2.$$

Total Sludge Solid Waste (Q_{TSW})(tons)

$$Q_{TSW}(dry) = Q_{urlimestone} + Q_{calcium\ sulfite} + Q_{calcium\ sulfate},$$

$$Q_{TSW}(dry) = 2.3485\ SO_2,$$

$$Q_{TSW}(wet) = Q_{TSW}(dry) \cdot \frac{100}{(100-m)},$$

$$Q_{TSW}(wet) = 4.697\ SO_2.$$

where

m = moisture content of solid waste (%),

2B.1.4 Double Alkali Wet Scrubbing. The equations are identical to the lime scrubber, but there is an additional amount of solid waste due to soda-ash makeup to the absorbent. The absorbent utilization also differs and so the coefficients are as follows:

$$Q_{lime} = 0.925\ SO_2,$$

$$Q_{urlimestone} = 0.0829\ SO_2,$$

$$Q_{calcium\ sulfite} = 1.518\ SO_2,$$

$$Q_{calcium\ sulfate} = 0.675\ SO_2.$$

Soda Ash Makeup ($Q_{soda\ ash}$) (tons)

$$Q_{soda\text{-}ash} = SO_2 \cdot SA \cdot \frac{MW\ soda\text{-}ash}{MW\ SO_2},$$

where

SA = Soda-ash makeup (fraction) molar basis,

$Q_{soda\text{-}ash} = 0.05\ SO_2$ tons.

Total Sludge Solid Waste (Q_{TSW}) (tons)

$$Q_{TSW}(\text{dry}) = Q_{\text{urlimestone}} + Q_{\text{calcium sulfite}}$$

$$+ Q_{\text{calcium sulfate}} + Q_{\text{soda-ash}},$$

$$Q_{TSW}(\text{dry}) = 2.3259\ SO_2,$$

$$Q_{TSW}(\text{wet}) = Q_{TSW}(\text{dry}) \cdot \frac{100}{(100-m)},$$

$$Q_{TSW}(\text{wet}) = 4.6518\ SO_2.$$

2B.1.5 Magnesium Oxide. Solid waste comes from absorbent makeup (process solid waste) and from the loss in separation (regeneration solid waste).

Process Solid Waste ($Q_{\text{magnesium oxide}}$) (tons)

$$Q_{\text{magnesium oxide}} = SO_2 \cdot AB \cdot \frac{\text{MW magnesium oxide}}{\text{MW } SO_2} \text{ tons},$$

$$Q_{\text{magnesium oxide}} = 0.01875\ SO_2.$$

where

SO_2 = quantity of SO_2 captured (tons),

AB = absorbent makeup (fraction) molar basis.

Regeneration Solid Waste ($Q_{\text{magnesium sulfite}}$) (tons)

$$Q_{\text{magnesium sulfite}} = SO_2 \cdot SL \cdot \frac{\text{MW magnesium sulfite}}{\text{MW } SO_2},$$

$$Q_{\text{magnesium sulfite}} = 0.08125\ SO_2.$$

where

SL = separation loss.

Total Sludge Solid Waste (Q_{TSW}) (tons)

$$Q_{TSW}(dry) = Q_{magnesium\ oxide} + Q_{magnesium\ sulfite},$$

$$Q_{TSW}(dry) = 0.01\ SO_2,$$

$$Q_{TSW}(wet) = Q_{TSW}(wet) \cdot \frac{100}{(100-m)},$$

$$Q_{TSW}(wet) = 0.1539\ SO_2.$$

where

m = moisture content of solid waste (%).

2B.1.6 Wellman-Lord. The equations are the same as for magnesium oxide except that sodium sulfite (Na_2SO_3) is used as the absorbent and sodium bisulfite ($NaHSO_3$) is produced.

Process Solid Waste ($Q_{sodium\ sulfite}$) (tons)

$$Q_{sodium\ sulfite} = SO_2 \cdot AB \cdot \frac{MW\ sodium\ sulfite}{MW\ SO_2},$$

$$Q_{sodium\ sulfite} = 0.059\ SO_2.$$

Regeneration Solid Waste ($Q_{sodium\ bisulfite}$) (tons)

$$Q_{sodium\ bisulfite} = SO_2 \cdot SL \cdot \frac{MW\ sodium\ bisulfite}{MW\ SO_2},$$

$$= 0.08125\ SO_2.$$

Total Sludge Solid Waste (Q_{TSW}) (tons)

$$Q_{TSW}(dry) = Q_{sodium\ sulfite} + Q_{sodium\ bisulfite},$$

$$Q_{TSW}(dry) = 0.14025\ SO_2,$$

$$Q_{TSW}(wet) = Q_{TSW}(dry) \cdot \frac{100}{(100-m)},$$

$$Q_{TSW}(wet) = 0.2158SO_2.$$

where

m = moisture content of solid waste (%),

2B.2 Equations Used To Calculate Quantity of FGD Sludge and Its Major Components for Dry Sorbent Injection

All assumptions and equations are from Reference 13. Table 2B.2 sets out the chemical formulae and molecular weights used. The desulfurization occurs via four reactions.

$$2\ NaHCO_3 + SO_2 \rightleftharpoons Na_2SO_3 + CO_2 + H_2O + O_2$$

$$2\ NaHCO_3 \rightleftharpoons Na_2CO_3 + H_2O + CO_2$$

$$Na_2CO_3 + SO_2 \longrightarrow Na_2SO_3 + CO_2$$

$$Na_2SO_3 + 1/2O_2 \longrightarrow Na_2SO_4$$

2B.2.1 Quantity of Sodium Bicarbonate (Nahcolite) Required

From the equations, 2 moles of $NaHCO_3$ are required to react with one mole of SO_2

$$Q_{nahcolite} = SO_2 \cdot R \cdot 2\frac{1}{U} \cdot \frac{MWNaHCO_3}{MWSO_2}$$

$$Q_{nahcolite} = 3.75\ SO_2.$$

where

SO_2 = quantity of SO_2 captured (tons) (see Section 2B1.1),

R = stoichiometric ratio: moles SO_2:moles nahcolite (assumed to be 1:1),

U = absorbent utilization (fraction) molar basis (assumed to be 0:70).

2B.2.2 Solid Waste Produced

The spent nahcolite in fact weighs less than the original sorbent because of the evolution of CO_2 and H_2O during the reaction with SO_2. The reduction is about 18%. The total solid waste (Q_{TSW}) is, therefore,

$Q_{TSW} = 3.075\ SO_2$.

The solid waste is made up of approximately 1.5% sodium bicarbonate, 25.4% sodium carbonate, 52.2% sodium sulfite, and 20.9% sodium sulfate.

The coefficients are therefore:

Sodium bicarbonate	0.046 SO_2
Sodium carbonate	0.781 SO_2
Sodium sulfite	1.605 SO_2
Sodium sulfate	0.643 SO_2

APPENDIX 2C

DESCRIPTION OF COMPUTER MODULE

The coal-fired power plant computer module consists of a series of five subroutines:BURN, PRECIP, FGDS, OPRINT, and ERRCH. The first three of these are subroutines for each of the three stages in a power plant system - the burner (boiler), precipitator, and FGD systems. The last two are used for output printing and error checks. The module is set to work by a call to subroutine BURN,

CALL BURN (C, BOT, FA, SLUD, GAS, IBLR, IPREC, IFGD, PREFF, SO2EFF, Q),

where

C = vector of size 50 with input characteristics of the coal, used for input only (not overwritten);

BOT, FA,
SLUD, GAS = vectors of size 50 with the output characteristics of the bottom ash, fly ash, FGD sludge, and stack gas, respectively. These vectors are used for output only;

IBLR = boiler type;

IPREC = precipitator indicator. 1 means there is a precipitator before the FGD system (if any), IPREC = 0 means the FGD system is used as a precipitator to collect fly ash;

PREFF = the efficiency of the precipitator in removing fly ash, in percent;

SO2EFF = the efficiency of the FGD system in removing SO_2;

Q = quantity of coal.

After calling BURN, the other subroutines will be called internally.

The module has one common block, CBURN, of size 255, which is in all of the subroutines.

All of the systems' coefficients (except for lime and limestone in FGDS, below) are in terms of amount of material passing through the respective system, although in the module sometimes the amount of material captured is calculated first. Almost all of the coefficients are read in from a data file, except those that are dependent upon some input value. These will be noted in the description of each subroutine, below.

Subroutine BURN

BURN first sends the calling parameters to ERRCH to check for input errors. It then reads the input coal characteristics into the first 50 elements of CBURN. The composition of the bottom ash and pass-through of all relevant materials are then calculated using the coefficients for the appropriate boiler from the data file. BURN then calls PRECIP, FGDS, and OPRINT.

Special Notes:

1) All sulfur not in the bottom ash is assumed to change to SO_2 on output (array element 35 (AE35)).
2) All carbon not in the bottom ash is assumed to change to CO_2 on output (AE42).
3) AE36 to AE38 (NO_2,CO,CH_4) are calculated using the total input quantity of coal.
4) The array STACK contains the emissions from the boiler not including the bottom ash. Hereafter, STACK will be the input to and output

from the other system subroutines. Upon output from FGDS, whatever is in STACK is what is considered to go up the power plant stack. BASH contains the bottom ash output from the boiler.

Subroutine PRECIP

PRECIP has all of its pass-through coefficients for ash and trace elements calculated on the basis of precipitator efficiency input. AE36 to AE38 and AE42 are assumed to pass through the precipitator untouched and have a coefficient of 1. Sulfur and sludge components are disregarded at this time and have coefficient values of 0.

Special Notes:

1) PRECIP is called even if IPREC = 0. If this is the case, the fly ash components are brought into FGDS and used as the respective entries in the sludge output vector.
2) FLY is the fly ash output vector from the precipitator.

Subroutine FGDS

FGDS calculates the amount of ash, trace elements, SO_2, and sludge components output from the FGD system.

Special Notes:

1) If there is no precipitator before the FGD system, the values for ash and the trace elements are taken to be the amount calculated in PRECIP. Therefore, the elements in FGD (the sludge output vector) are equated with the respective elements of FLY, and those elements of FLY are set to 0.

2) Sludge components (AE25 to AE33 and AE43 to AE45) are calculated using the amount of SO_2 captured in the system.

3) The captured SO_2 is determined by SO2EFF, the input FGD system efficiency.

4) No coefficients are available for the amounts of some of the trace elements contained in the FGD system lime and limestone. These elements are given a coefficient of 0 in LIME or LIMES, and are noted in the output.

Subroutine OPRINT

OPRINT is used to print the output.

Subroutine ERRCH

ERRCH checks that all calling parameters for subroutine BURN are within their correct range and that the sum of the input coal characteristics is not greater than the total quantity of coal. If there are any errors, no calculations are done and control is returned to the calling program.

After all calculations have been made, the output vectors BASH, FLY, FGD, and STACK (which are all within common block CBURN) are equated with other vectors not in the block (BOT, FA, SLUD, and GAS, respectively), and these vectors are passed back to the calling program.

APPENDIX 2D

COMPUTER CODE AND SAMPLE OUTPUT

This section sets out the computer code used for the coal combustion module with a sample input and the resulting output. Table 2D.1 gives the coal characteristics used as input. The other input variables used were as follows:

Quantity of coal (Q) = 100,000.0 tons

Precipitator efficiency (PREFF) = 99.0%

SO_2 removal (SO2EFF) = 85.0%

Lime wet scrubbing system (IFGD) = 1

Precipitator employed (IPREC) = 1

Large pulverized boiler (IBLR) = 1

The calling program of the code is used only to set the input variables.

In some cases data may be missing and so the output is incomplete. An asterisk is used to indicate cases where there were no data on the quantity of an element in the scrubbing media. This means that the amount of the trace element in the FGD sludge may be understated.

Table 2D.1
Input Characteristics of Coal

Element	Input Quantity (tons)	Element	Input Quantity (tons)
Ash	9200.0	Manganese	20.0
Sulfur	1600.0	Mercury	0.014
Antimony	0.08	Nickel	1.5
Arsenic	1.1	Selenium	0.35
Beryllium	0.2	Silver	0.02
Cadmium	0.03	Thallium	0.02
Chromium	1.5	Zinc	1.28
Copper	1.6	Uranium	0.1
Iron	1000.0	Thorium	0.28
Lead	1.09	Carbon	72,000.0
Magnesium	52.0		

```
      PROGRAM CT(INPUT,OUTPUT,TAPE1,TAPE9=OUTPUT)
      DIMENSION COAL(50),BASH(50),FLY(50),STACK(50),FGD(50)
      Q=100000.00
      PREFF=99.
      SO2EFF=85.
      IFGD=1
      IPREC=1
      IBLR=1
      COAL(1)=9200.
      COAL(2)=1600.
      COAL(3)=0.08
      COAL(4)=1.1
      COAL(5)=0.2
      COAL(6)=0.03
      COAL(7)=1.5
      COAL(8)=1.6
      COAL(9)=1000.0
      COAL(10)=1.09
      COAL(11)=52.0
      COAL(12)=20.0
      COAL(13)=0.014
      COAL(14)=1.5
      COAL(15)=0.35
      COAL(16)=0.02
      COAL(17)=0.02
      COAL(18)=1.28
      COAL(19)=0.1
      COAL(20)=0.28
      COAL(21)=0.
      COAL(22)=0.
      COAL(23)=0.
      DO 6 I=24,38
      COAL(I)=0.
    6 CONTINUE
      COAL(39)=800.
      COAL(40)=72000.
      COAL(41)=8000000.
      DO 7 I=42,50
      COAL(I)=0.
    7 CONTINUE
      CALL BURN(COAL,BASH,FLY,FGD,STACK,IBLR,IPREC,IFGD,PREFF,SO2EFF,Q)
      STOP
      END
```

```
      SUBROUTINE BURN(C,BOT,FA,SLUD,GAS,IBLR,IPREC,IFGD,PREFF,SO2EFF,Q)
      COMMON/CBURN/COAL(50),FLY(50),BASH(50),FGD(50),STACK(50),
     -STAR(3,23)
      REAL BCHAR(4,50),C(50),BOT(50),FA(50),SLUD(50),GAS(50)
C   * COEFFICIENTS READ IN TO GIVE SPLIT BETWEEEN BOTTOM ASH
C   * AND FLY ASH
      READ(1,1001)((BCHAR(I,J),J=1,50),I=1,4)
1001  FORMAT(10F7.5)
C   * USED TO STORE COAL CHARACTERISTICS FOR WRITING ON OUTPUT
      DO 30 I=1,50
      COAL(I)=C(I)
   30 CONTINUE
C   * CALCULATION OF RA-226,RA-228 & PB-210 IF NOT GIVEN AS INPUT DATA
      IF(COAL(21) .EQ. 0.)COAL(21)=(3.38E-7)*COAL(19)
      IF(COAL(22) .EQ. 0.)COAL(22)=(4.01E-10)*COAL(20)
      IF(COAL(23) .EQ. 0.)COAL(23)=(4.37E-9)*COAL(19)
      CALL ERRCH(IBLR,IPREC,IFGD,PREFF,SO2EFF,ICHECK,Q)
      IF(ICHECK .EQ. 1)GO TO 500
C   * CALCULATION OF ELEMENT SPLIT BETWEEN BOTTOM AND FLY ASH
      DO 10 I=1,34
      STACK(I)=BCHAR(IBLR,I)*COAL(I)
      BASH(I)=COAL(I)-STACK(I)
   10 CONTINUE
C   * CONVERSION OF SULFUR IN STACK GAS TO SO2
      STACK(35)=BCHAR(IBLR,35)*STACK(2)
      STACK(2)=0.
C   * CALCULATION OF NO2,CO & CH4 IN STACK GAS
      DO 20 J=36,38
      STACK(J)=Q*BCHAR(IBLR,J)
      BASH(J)=0.
   20 CONTINUE
C   * CALCULATION OF PYRITIC SULFUR IN BOTTOM ASH
      STACK(39)=BCHAR(IBLR,39)*COAL(39)
      BASH(39)=COAL(39)-STACK(39)
      STACK(39)=0.
C   * CALCULATION OF CARBON SPLIT BETWEEN BOTTOM ASH AND STACK GAS
      STACK(40)=BCHAR(IBLR,40)*COAL(40)
      BASH(40)=COAL(40)-STACK(40)
C   * BTU OUTPUT SET TO ZERO
      STACK(41)=0.
      BASH(41)=0.
C   * CONVERSION OF CARBON IN STACK GAS TO CO2
      STACK(42)=BCHAR(IBLR,42)*STACK(40)
      BASH(42)=0.
      STACK(40)=0.
      BASH(35)=0.
      DO 50 I=43,50
      BASH(I)=0.
      STACK(I)=BCHAR(IBLR,I)*COAL(I)
   50 CONTINUE
      CALL PRECIP(IPREC,PREFF)
      CALL FGDS(IPREC,IFGD,SO2EFF)
      CALL OPRINT
      DO 40 I=1,50
      BOT(I)=BASH(I)
      FA(I)=FLY(I)
      SLUD(I)=FGD(I)
      GAS(I)=STACK(I)
   40 CONTINUE
  500 RETURN
      END
```

```
      SUBROUTINE PRECIP(IPREC,PREFF)
C    * CALCULATES THE AMOUNT OF EACH ELEMENT CAPTURED IN THE PRECIPITATOR
      COMMON/CBURN/COAL(50),FLY(50),BASH(50),FGD(50),STACK(50),
     -STAR(3,23)
      DIMENSION PREC(50)
      DATA PREC/34*0.,16*1./
      DO 30 I=1,3
      DO 20 J=1,23
      STAR(I,J)=3H
   20 CONTINUE
   30 CONTINUE
C    * CALCULATION OF FRACTION OF EACH ELEMENT WHICH PASSES THROUGH
C    * THE PRECIPITATOR AS A FUNCTION OF PRECIPITATOR EFFICIENCY
      PREC(1)=(100.-PREFF)/100.
      PREC(3)=25.84*ALOG(100.*PREC(1)+1.)/100.
      PREC(4)=6.84*ALOG(100.*PREC(1)+1.)/100.
      PREC(5)=1.*PREC(1)
      PREC(6)=15.23*ALOG(100.*PREC(1)+1.)/100.
      PREC(7)=2.05*PREC(1)
      PREC(8)=1.25*PREC(1)
      PREC(9)=1.*PREC(1)
      PREC(10)=19.19*ALOG(100.*PREC(1)+1.)/100.
      PREC(11)=1.*PREC(1)
      PREC(12)=1.*PREC(1)
      PREC(13)=.975
C    * CALCULATION OF PASS THROUGH FOR HG IF FGD SYSTEM ONLY USED
      IF(IPREC .EQ. 0)PREC(13)=.87
      PREC(14)=2.33*PREC(1)
      PREC(15)=20.84*ALOG(100.*PREC(1)+1.)/100.
      PREC(16)=.582*PREC(1)
      PREC(17)=2.69*PREC(1)
      PREC(18)=1.73*PREC(1)
      PREC(19)=1.97*PREC(1)
      PREC(20)=.86*SQRT(100.*PREC(1))/100.
      PREC(21)=1.5*PREC(1)
      PREC(22)=1.5*PREC(1)
      PREC(23)=19.19*ALOG(100.*PREC(1)+1.)/100.
C    * CALCULATION OF ELEMENT SPLIT BETWEEN PRECIPITATOR AND STACK GAS
      DO 10 I=1,50
      FLY(I)=STACK(I)-STACK(I)*PREC(I)
      STACK(I)=STACK(I)-FLY(I)
   10 CONTINUE
      RETURN
      END
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      SUBROUTINE FGDS(IPREC,IFGD,SO2EFF)
C   * CALCULATES MAJOR COMPONENTS AND TRACE ELEMENTS IN FGD SLUDGE
      COMMON/CBURN/COAL(50),FLY(50),BASH(50),FGD(50),STACK(50),
     -STAR(3,23)
      REAL FGDC(9,50),LIME(23),LIMES(23)
C   * READS FROM DATA FILE INPUT FRACTIONS OF TRACE ELEMENTS
C   * IN LIME AND LIMESTONE RESPECTIVELY
      READ(1,1001)(LIME(I),I=1,23),(LIMES(I),I=1,23)
C   * READS IN COEFFICIENTS TO CALCULATE THE AMOUNT OF EACH
C   * ELEMENT IN SLUDGE FOR EACH TYPE OF FGD SYSTEM
      READ(1,1002)((FGDC(I,J),J=1,50),I=1,9)
1001 FORMAT(7E10.3/7E10.3/7E10.3/2E10.3)
1002 FORMAT(10F7.5)
      IF(IFGD .EQ. 9)SO2EFF=0.
      FGDC(IFGD,35)=SO2EFF/100.
      IF(IPREC .EQ. 1)GO TO 5
C   * IF FGD ALSO USED AS PRECIPITATOR, THE SAME FRACTION OF
C   * EACH ELEMENT  AS WOULD  BE CAPTURED IN A PRECIPITATOR IS
C   * ASSUMED CAPTURED IN THE FGD SYSTEM AND APPEARS IN THE SLUDGE
      DO 4 I=1,24
      FGD(I)=FLY(I)
      FLY(I)=0.
    4 CONTINUE
      GO TO 6
C   * CALCULATION OF COAL TRACE ELEMENT SPLIT BETWEEN SLUDGE AND
C   * STACK GAS WHEN A PRECIPITATOR IS USED PRIOR TO THE FGD SYSTEM
    5 DO 10 I=1,24
      FGD(I)=STACK(I)-STACK(I)*FGDC(IFGD,I)
      STACK(I)=STACK(I)-FGD(I)
      IF(I .EQ. 1)GO TO 10
C   * FOR REGENERABLE SCRUBBERS THE WASTE CONSISTS ONLY OF
C   * AN 8% REGENERATION LOSS
      IF(IFGD .EQ. 4 .OR. IFGD .EQ. 5)FGD(I)=.08*FGD(I)
   10 CONTINUE
C   * CALCULATION OF SO2 SPLIT BETWEEN SLUDGE AND STACK GAS
    6 FGD(35)=STACK(35)*FGDC(IFGD,35)
      STACK(35)=STACK(35)-FGD(35)
      IF(IFGD .EQ. 9)GO TO 7
      IF(IFGD .EQ. 8)GO TO 7
      IF(IFGD .EQ. 4 .OR. IFGD .EQ. 5)GO TO 7
      IF(IFGD .EQ. 2 .OR. IFGD .EQ. 7)GO TO 8
C   * CALCULATION OF QUANTITY OF LIME REQUIRED FOR DOUBLE ALKALI
      IF(IFGD .EQ. 3)QLIME=.925*FGD(35)
C   * CALCULATION OF LIME REQUIRED BY A LIME SCRUBBER
      IF(IFGD .EQ. 1 .OR. IFGD .EQ. 6)QLIME=.975*FGD(35)
C   * CALCULATION OF TRACE ELEMENTS IN SLUDGE FROM LIME
C   * IF NO DATA AVAILABLE OUTPUT PRINTS ***
      DO 9 I=3,23
      FGD(I)=FGD(I)+QLIME*LIME(I)
      IF(LIME(I) .EQ. 0.)STAR(2,I)=3H*
    9 CONTINUE
      GO TO 7
C   * CALCULATION OF QUANITY OF LIMESTONE USED IN LIMESTONE
C   * SCRUBBER AND TRACE ELEMENTS FROM LIMESTONE IN SLUDGE
    8 QLIMES=1.7625*FGD(35)
      DO 11 I=3,23
      FGD(I)=FGD(I)+QLIMES*LIMES(I)
      IF(LIMES(I) .EQ. 0.)STAR(2,I)=3H*
   11 CONTINUE
C   * CALCULATION OF MAJOR COMPONENTS OF THE FGD SLUDGE
    7 DO 20 I=25,33
      FGD(I)=FGD(35)*FGDC(IFGD,I)
C   * CALCULATION OF TOTAL WASTE- WET ASH  + WET SLUDGE
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```
      IF(I .EQ. 25)FGD(I)=FGD(35)*FGDC(IFGD,I)+2.*FGD(1)
C   * CALCULATION OF TOTAL WASTE WET ASH + WET SLUDGE FOR
C   * REGENERABLE SCRUBBERS
      IF(I .EQ. 25 .AND. (IFGD .EQ. 4 .OR. IFGD .EQ. 5))FGD(I)=
     -FGD(35)*FGDC(IFGD,I)+1.35*FGD(1)
C   * CALCULATION OF TOTAL WASTE FOR DRY SCUBBER - DRY SLUDGE
C   * + DRY ASH
      IF(I .EQ. 25 .AND. IFGD .EQ. 8)FGD(I)=FGD(35)*FGDC(IFGD,I)+
     -FGD(1)
   20 CONTINUE
C   * CALCULATION OF WATER IN FGD WASTE
      FGD(34)=FGD(35)*FGDC(IFGD,34)+FGD(1)
      IF(IFGD .EQ. 4 .OR. IFGD .EQ. 5)FGD(34)=FGD(35)*FGDC(IFGD,34)+
     -.35*FGD(1)
      IF(IFGD .EQ. 8)FGD(34)=0.
      DO 30 I=36,38
      FGD(I)=0.
   30 CONTINUE
      DO 40 I=39,50
      FGD(I)=FGDC(IFGD,I)*FGD(35)
   40 CONTINUE
      RETURN
      END



      SUBROUTINE OPRINT
      COMMON/CBURN/COAL(50),FLY(50),BASH(50),FGD(50),STACK(50),
     -STAR(3,23)
      WRITE(9,910)(COAL(I),BASH(I),FLY(I),STAR(1,I),
     -FGD(I),STAR(2,I),STACK(I),STAR(3,I),I=1,12)
      WRITE(9,914)(COAL(I),BASH(I),FLY(I),STAR(1,I),FGD(I),
     -STAR(2,I),STACK(I),STAR(3,I),I=13,23)
      WRITE(9,913)(COAL(I),BASH(I),FLY(I),FGD(I),STACK(I),I=24,30)
      WRITE(9,911)(COAL(I),BASH(I),FLY(I),FGD(I),STACK(I),I=31,38)
      WRITE(9,915)(COAL(I),BASH(I),FLY(I),FGD(I),STACK(I),I=39,45)
      WRITE(9,916)(COAL(I),BASH(I),FLY(I),FGD(I),STACK(I),I=46,50)
      WRITE(9,912)
  910 FORMAT(1X,*COMPONENT*,T30,*INPUT COAL*,T45,*BOTTOM ASH*,T60,*FLY A
     -SH*,T75,*FGD SLUDGE*,T90,*STACK GAS*/1X,12(*-*),T30,12(*-*),T45,
     -12(*-*),T60,12(*-*),T75,12(*-*),T90,12(*-*)/
     -1X,*ASH*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*SULFUR*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*ANTIMONY*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*ARSENIC*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*BERYLLIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*CADMIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*CHROMIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*COPPER*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*IRON*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*LEAD*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*MAGNESIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
     -1X,*MANGANESE*,T30,2(E12.3,3X),3(E12.3,A3))
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```
914 FORMAT(1X,*MERCURY*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*NICKEL*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*SELENIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*SILVER*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*THALLIUM*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*ZINC*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*URANIUM-238*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*THORIUM-232*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*RADIUM-226*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*RADIUM-228*,T30,2(E12.3,3X),3(E12.3,A3)/
   -1X,*LEAD-210*,T30,2(E12.3,3X),3(E12.3,A3))
913 FORMAT(1X,*HYDROCARBONS*,
   -T30,5(E12.3,3X)/1X,*TOTAL FGD SLUDGE*,T30,5(E12.3,3X)/1X,
   -*UNREACTED LIMESTONE*,
   -T30,5(E12.3,3X)/1X,*CALCIUM SULFITE*,T30,5(E12.3
   -,3X)/1X,*CALCIUM SULFATE*,T30,5(E12.3,3X)/1X,*SODA-ASH*,T30,
   -5(E12.3,3X)/1X,*MAGNESIUM SULFITE*,T30,5(E12.3,3X))
911 FORMAT(1X,*MAGNESIUM OXIDE*,T30,5(E12.3,3X)/
   -1X,*SODIUM BISULFITE*,T30,5(E12.3,3X)/
   -1X,*SODIUM SULFITE*,T30,5(E12.3,3X)/
   -1X,*WATER*,T30,5(E12.3,3X)/
   -1X,*SULFUR DIOXIDE*,T30,5(E12.3,3X)/
   -1X,*NITROUS OXIDES*,T30,5(E12.3,3X)/
   -1X,*CARBON MONOXIDE*,T30,5(E12.3,3X)/
   -1X,*METHANE*,T30,5(E12.3,3X))
915 FORMAT(1X,*PYRITIC SULFUR*,T30,5(E12.3,3X)/
   -1X,*CARBON*,T30,5(E12.3,3X)/
   -1X,*BTU CONTENT*,T30,5(E12.3,3X)/
   -1X,*CARBON DIOXIDE*,T30,5(E12.3,3X)/
   -1X,*SODIUM BICARBONATE*,T30,5(E12.3,3X)/
   -1X,*SODIUM CARBONATE*,T30,5(E12.3,3X)/
   -1X,*SODIUM SULFATE*,T30,5(E12.3,3X))
916 FORMAT(1X,*EMPTY*,T30,5(E12.3,3X)/
   -1X,*EMPTY*,T30,5(E12.3,3X)/
   -1X,*EMPTY*,T30,5(E12.3,3X)/
   -1X,*EMPTY*,T30,5(E12.3,3X)/
   -1X,*EMPTY*,T30,5(E12.3,3X)/)
912 FORMAT(1X,1H*,*ACTUAL QUANTITY UNCERTAIN DUE TO UNKNOWN AMOUNT ADD
   -ED FROM LIME/LIMESTONE IN FGD SCRUBBER.*/)
    RETURN
    END
```

```
      SUBROUTINE ERRCH(IBLR,IPREC,IFGD,PREFF,SO2EFF,ICHECK,Q)
C   * USED TO ENSURE INPUT DATA WITHIN CORRECT BOUNDS
      COMMON/CBURN/COAL(50)
      ICHECK=0
C   * BOILER TYPE MUST BE AN INTEGER FIGURE BETWEEN 1 AND 4
      DO 10 I=1,4
      IF(IBLR .EQ. I)GO TO 20
   10 CONTINUE
      ICHECK=1
      WRITE(9,901)IBLR
C   * IPREC FLAG IS EITHER 0 FOR NO PRECIPITATOR OR 1 FOR PRECIPITATOR
   20 IF(IPREC .EQ. 0 .OR. IPREC .EQ. 1)GO TO 40
      ICHECK=1
      WRITE(9,902)IPREC
C   * FGD SYSTEM INPUT INTEGER BETWEEN 1 AND 9 AND MUST BE
C   * COMPATIBLE WITH PRECIPITATOR OR NO PRECIPITATOR
   40 DO 60 I=1,9
      IF(IFGD .NE. I)GO TO 60
      IF(IFGD .LE. 5 .AND. IPREC .EQ. 1)GO TO 50
      IF(IFGD .EQ. 9 .AND. IPREC .EQ. 1)GO TO 50
      IF(IFGD .GE. 6 .AND. IPREC .EQ. 0)GO TO 50
   60 CONTINUE
      ICHECK=1
      WRITE(9,904)
C   * PRECIPITATOR EFFICIENCY MUST BE BETWEEN 0 AND 100%
   50 IF(PREFF .GE. 0. .AND. PREFF .LE. 100.)GO TO 70
      ICHECK=1
      WRITE(9,905)
C   * SO2 REMOVAL RATE MUST BE BETWEEN 0 AND 100%
   70 IF(SO2EFF .GE. 0. .AND. SO2EFF .LE. 100.)GO TO 80
      ICHECK=1
      WRITE(9,906)
C   * SUM OF ELEMENTS IN COAL CANNOT BE GREATER THAN TOTAL
C   * QUANTITY OF COAL
   80 CSUM=0.
      DO 90 I=1,24
      CSUM=CSUM+COAL(I)
   90 CONTINUE
      IF(Q .GE. CSUM)GO TO 100
      ICHECK=1
      WRITE(9,907)
C   * IF ICHECK=1 NO CALCULATIONS MADE AND ERROR MESSAGE PRINTED
  901 FORMAT(1X,*THERE IS NO BOILER TYPE*,I3//)
  902 FORMAT(1X,I3,1X,*IS NOT A VALID PRECIPITATOR PARAMETER (ONLY 0 OR
     -1).*//)
  904 FORMAT(1X,*YOU HAVE ENTERED AN INCORRECT FGD TYPE OR AN INCORRECT
     -PRECIPITATOR/FGD PARAMETER MATCHUP*/)
  905 FORMAT(1X,*PRECIPITATOR EFFICIENCY IS NOT IN THE INTERVAL (0,100).
     -*//)
  906 FORMAT(1X,*FGD SYSTEM SO2 REMOVAL EFFICIENCY IS NOT IN THE INTERVA
     -L (0,100).*//)
  907 FORMAT(1X,*THE SUM OF THE CHARACTERISTICS OF THE INPUT COAL IS GRE
     -ATER THAN THE TOTAL INPUT COAL.*//)
  100 RETURN
      END
```

```
 .80000 .95000 .94830 .98000 .83710 .28180 .87800 .87450 .76140 .94350
 .82550 .84660 .98720 .84220 .98820 .94490 .88070 .88630 .69970 .80190
 .80000 .80000 .943501.000001.000001.000001.000001.000001.000001.00000
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1.000003.670000.000000.000000.000000.000000.000000.000000.000000.00000
 .40000 .95000 .91660 .82710 .41800 .81440 .54150 .68920 .39460 .92560
 .37860 .37220 .98770 .73770 .80660 .78000 .97390 .92880 .54240 .38740
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1.000001.000001.000001.000002.00000 .00750 .00100 .00500 .95000 .98000
1.000003.670000.000000.000000.000000.000000.000000.000000.000000.00000
 .10000 .95000 .91660 .82710 .41800 .81440 .54150 .68920 .39460 .92560
 .37860 .37220 .98770 .73770 .80660 .78000 .97390 .92880 .54240 .38740
 .10000 .10000 .925601.000001.000001.000001.000001.000001.000001.00000
1.000001.000001.000001.000002.00000 .00300 .00500 .00150 .95000 .98000
1.000003.670000.000000.000000.000000.000000.000000.000000.000000.00000
 0.        0.        0.         .150E-05  .180E-08  .337E-07  .312E-05
  .190E-05  .627E-07  .207E-06  .768E-02  .155E-03 0.        0.
  .174E-04 0.        0.         .196E-03 0.        0.        0.
 0.        0.
 0.        0.        0.         .171E-05  .187E-06  .155E-06  .814E-05
  .169E-05  .627E-07  .129E-05  .768E-02  .155E-03 0.        0.
  .827E-06 0.        0.         .108E-03 0.        0.        0.
 0.        0.
 .35000 .35000 .35000 .35000 .35000 .35000 .35000 .35000 .35000 .35000
 .35000 .35000 .87000 .35000 .35000 .35000 .35000 .35000 .35000 .35000
 .35000 .35000 .350000.000004.72800 .174001.51600 .674000.000000.00000
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 .35000 .35000 .87000 .35000 .35000 .35000 .35000 .35000 .35000 .35000
 .35000 .35000 .350000.000004.69700 .352501.36500 .631000.000000.00000
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 .35000 .35000 .87000 .35000 .35000 .35000 .35000 .35000 .35000 .35000
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0.000000.000000.000000.000000.000000.000000.000000.000000.000000.00000
```

COMPONENT	INPUT COAL	BOTTOM ASH	FLY ASH	FGD SLUDGE	STACK GAS
ASH	.920E+04	.184E+04	.729E+04	.478E+02	.258E+02
SULFUR	.160E+04	.800E+02	0.	0.	0.
ANTIMONY	.800E-01	.414E-02	.623E-01	.883E-02*	.476E-02
ARSENIC	.110E+01	.220E-01	.103E+01	.370E-01	.179E-01
BERYLLIUM	.200E+00	.326E-01	.166E+00	.109E-02	.586E-03
CADMIUM	.300E-01	.355E-02	.237E-01	.190E-02	.977E-03
CHROMIUM	.150E+01	.183E+00	.129E+01	.254E-01	.945E-02
COPPER	.160E+01	.201E+00	.138E+01	.162E-01	.612E-02
IRON	.100E+04	.239E+03	.754E+03	.495E+01	.266E+01
LEAD	.109E+01	.616E-01	.892E+00	.894E-01	.479E-01
MAGNESIUM	.520E+02	.907E+01	.425E+02	.196E+02	.150E+00
MANGANESE	.200E+02	.307E+01	.168E+02	.501E+00	.593E-01
MERCURY	.140E-01	.179E-03	.346E-03	.175E-02*	.117E-01
NICKEL	.150E+01	.237E+00	.123E+01	.191E-01*	.103E-01
SELENIUM	.350E+00	.413E-02	.296E+00	.763E-01	.175E-01
SILVER	.200E-01	.110E-02	.188E-01	.715E-04*	.385E-04
THALLIUM	.200E-01	.239E-02	.171E-01	.308E-03*	.166E-03
ZINC	.128E+01	.146E+00	.111E+01	.507E+00	.687E-02
URANIUM-238	.100E+00	.300E-01	.686E-01	.896E-03*	.482E-03
THORIUM-232	.280E+00	.555E-01	.223E+00	.126E-02*	.676E-03
RADIUM-226	.338E-07	.676E-08	.266E-07	.264E-09*	.142E-09
RADIUM-228	.112E-09	.225E-10	.885E-10	.876E-12*	.472E-12
LEAD-210	.437E-09	.247E-10	.357E-09	.356E-10*	.192E-10
HYDROCARBONS	0.	0.	0.	0.	0.
TOTAL FGD SLUDGE	0.	0.	0.	.123E+05	0.
UNREACTED LIMESTONE	0.	0.	0.	.450E+03	0.
CALCIUM SULFITE	0.	0.	0.	.392E+04	0.
CALCIUM SULFATE	0.	0.	0.	.174E+04	0.
SODA-ASH	0.	0.	0.	0.	0.
MAGNESIUM SULFITE	0.	0.	0.	0.	0.
MAGNESIUM OXIDE	0.	0.	0.	0.	0.
SODIUM BISULFITE	0.	0.	0.	0.	0.
SODIUM SULFITE	0.	0.	0.	0.	0.
WATER	0.	0.	0.	.616E+04	0.
SULFUR DIOXIDE	0.	0.	0.	.258E+04	.456E+03
NITROUS OXIDES	0.	0.	0.	0.	.900E+03
CARBON MONOXIDE	0.	0.	0.	0.	.500E+02
METHANE	0.	0.	0.	0.	.150E+02
PYRITIC SULFUR	.800E+03	.400E+02	0.	0.	0.
CARBON	.720E+05	.144E+04	0.	0.	0.
BTU CONTENT	.800E+07	0.	0.	0.	0.
CARBON DIOXIDE	0.	0.	0.	0.	.259E+06
SODIUM BICARBONATE	0.	0.	0.	0.	0.
SODIUM CARBONATE	0.	0.	0.	0.	0.
SODIUM SULFATE	0.	0.	0.	0.	0.
EMPTY	0.	0.	0.	0.	0.
EMPTY	0.	0.	0.	0.	0.
EMPTY	0.	0.	0.	0.	0.
EMPTY	0.	0.	0.	0.	0.
EMPTY	0.	0.	0.	0.	0.

*ACTUAL QUANTITY UNCERTAIN DUE TO UNKNOWN AMOUNT ADDED FROM LIME/LIMESTONE IN FGD SCRUBBER.

3 SOLID WASTE MODULE FOR ATMOSPHERIC FLUIDIZED BED COMBUSTION

3.1 Introduction

Atmospheric fluidized-bed combustion (AFBC) is an advanced combustion technique in which crushed coal burns in the presence of crushed limestone while held in suspension by upward-flowing combustion air. The technique has several advantages. Rapid heat transfer and high heat-release rates at a reduced temperature can be obtained, so that boiler tubes can be embedded in the combustion zone, resulting in smaller boilers. Fluidized-bed boilers can be fired with all grades of coal without serious modification. Further, the limestone acts as a sorbent to chemically remove SO_2 directly from the combustion zone, thus making AFBC an alternative to conventional combustion with FGD in order to comply with the stringent new SO_2 regulations.

Despite the advantages of the AFBC process, there are no commercial units now in operation. Industry representatives consider the boilers a high risk because their reliability and cost effectiveness for heavy loads have not been demonstrated.

3.2 General Description of a Utility AFBC Process

The DOE is sponsoring a program to develop conceptual designs for a nominal 600-MW utility AFBC steam generating plant in order to obtain the design information necessary for a demonstration effort. Three conceptual designs are being developed under this program by the following teams:

Burns and Roe/Combustion Engineering

Stone and Webster/Foster Wheeler Energy Corporation

Stone and Webster/Babcock and Wilcox

Although there are major differences between the three plans in the engineering details, the overall designs are very similar for the purpose of calculating the solid waste produced. Figure 3.1 is a schematic diagram of the AFBC boiler system used in the module.

The combustion of coal is carried out in two stages. The first stage is the main fluidized bed where most of the carbon is burned. The second stage is called the carbon burnup cell (CBC). The elutriated particles from the main bed are removed from the flue gas by the primary cyclone and returned to the CBC, where the combustion of the carbon present in these particles can take place. The elutriated particles can also be returned to the main bed. However, it is more difficult to obtain the same efficiency as with two stage combustion. All the proposed designs use a CBC[1].

The heat released by the burning of the feed coal is transferred to water/steam in tubes surrounding and submerged in the bed.

The flue gas streams from the main bed and CBC, after passing through cyclones, pass through an air heater where the input air to the main bed and CBC is heated to 600°F. The flue gas, after being cooled to about 250°F, passes through a baghouse filter for final cleaning.

This is the cleanup system proposed by Combustion Engineering and Foster Wheeler; at present, Babcock and Wilcox propose using electrostatic precipitators. Although this would help protect the air heater, it is an unproven ESP application. The collection could be hampered by the presence of calcium-based particulate components and also by low SO_2 concentrations in the flue gas[1].

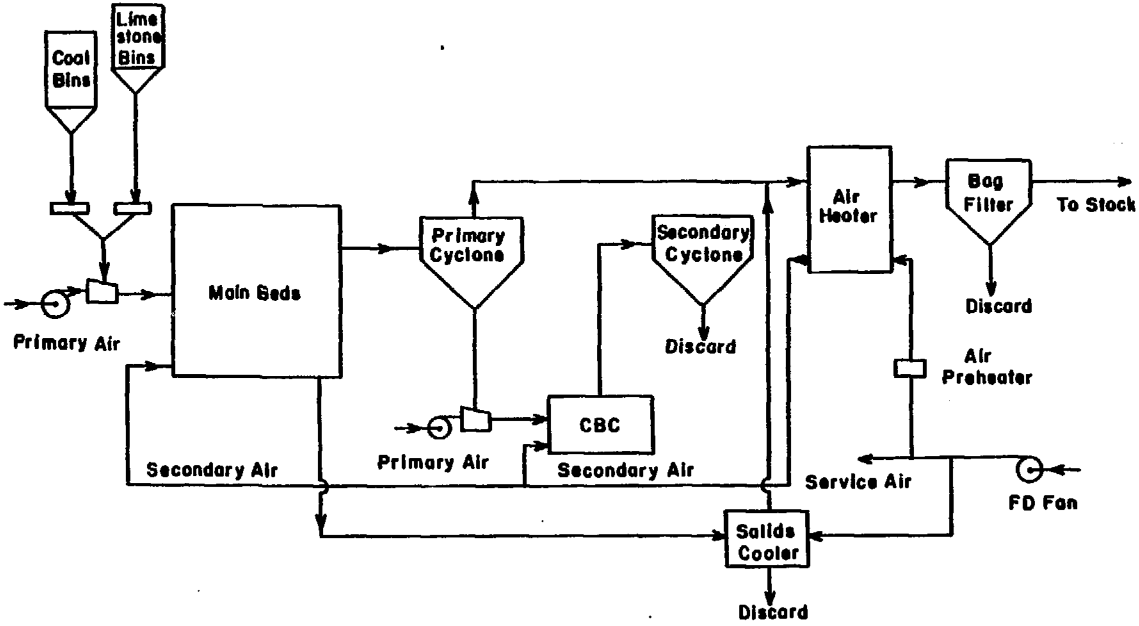

Figure 3.1 AFBC Conceptual Plant Design

The solids discharged from the main bed are discarded after recovering some of their sensible heat by cooling them with air. The solids obtained from the secondary cyclone and baghouse are also discarded.

The operating conditions of an AFBC process can vary widely and have a significant influence on the amount of solid waste produced. One influential variable is bed temperature, however, all three proposed designs assume 1550°F and 2000°F in the main bed and CBC, respectively[1].

The superficial velocity and bed height, or in other words the residence time, are critical as far as sulfur capture and limestone consumption are concerned. For the same sulfur removal the limestone requirement increases with increasing superficial velocity. In addition, the carbon consumption efficiency may decrease with increasing velocity. However, the bed area would be smaller if the velocity were larger. This would result in a smaller number of feeding points and possibly some saving in boiler cost.

3.3 Solid Waste Production

Fluidized-bed combustion produces two distinct types of solid waste, the elutriated fines that are captured by the particulate equipment and the coarser material that is extracted directly from the main bed drains. The spent bed material is expected to be composed mainly of $CaSO_4$, CaO, and inert mineral impurities in the limestone. The elutriated fines consist of ash, unburnt carbon, and spent bed material. There will be trace metals in all waste streams originating from both the coal and the limestone.

The total quantity of ash in the solid waste depends on the ash content of the coal and the efficiency of the precipitators, which is dictated by air pollution regulations. The amount of spent sorbent material depends on a much greater number of factors, including:

Fuel sulfur
Sulfur reduction required
Reactivity of the limestone
Particle size of the limestone
Bed temperature
Bed height
Bed velocity

A number of these factors can be "lumped" into a single operating parameter, the calcium to sulfur feed ratio (Ca/S), which greatly simplifies the calculation of the quantity of waste generated. At present, the only simple equation available, developed by IR&T[2], takes into account only sulfur removal rate, bed height, and bed velocity. Bed temperature is not included as a variable. However, this is expected to be reasonably constant amongst utility-sized AFBCs. The greatest weakness in the equation is that it is based on experiments conducted using only one type of limestone, and therefore differences in limestone reactivity are not taken into account. This can vary widely and will affect the Ca/S ratio. At present, however, there is no explanation as to why one limestone is more reactive than another, and no methods to predict reactivity have been developed[4]. Therefore, even with its limitations the equation would appear to be the best available.

The rate of elutriation of the waste from the main bed will vary depending on the operating conditions of the AFBC. For the module, the assumptions given in the Combustion Engineering design are used[3].

100 % input coal ash

40 % spent bed material

10 % input coal carbon

An elutriation rate of 40 % for the spent material is assumed for all present designs[1]. Combustion Engineering and Foster Wheeler both assume 100 % elutriation of the ash; Babcock and Wilcox assumes 75 %[1].

The quantity of the elutriated waste captured will depend on the efficiency of the collection devices. In the module the two cyclones will have pre-set removal rates of 90 % and 80 %, respectively. These are the figures used in Combustion Engineering's design[3]. The material collected in the first cyclone goes to the CBC, while that from the second cyclone is discarded as waste. The final baghouse collector will be of varying efficiency. The efficiency will be set internally in the module depending on the loading and the final allowable emissions to comply with air regulations. The allowable emissions will be given as an input.

The carbon balance depends on the combustion efficiency and the module assumes 90 % efficiency in both the main bed and the CBC. These figures are from the Combustion Engineering design[3].

The solid waste streams will contain trace metals from both the coal and the limestone. However, no complete data are yet available on the distribution of the trace metals between the different waste streams. Little work has been done concerning the fate of trace metals during AFB combustion, and no satisfactory estimate of the constituents of the AFB waste can be projected[5]. A survey was made of the National Technical Inforamtion Service (NTIS) abstracts for the last three years, and very few reports were found which addressed the problem. Swift and Vogel of ANL have looked at the fate of trace elements during fluidized-bed combustion using a pressurized system[6]. Trace element measurements have been made by members of the Lovelace Research Institute using the Morgantown Energy Research atmospheric fluidized bed,[7] but only the concentrations of trace elements are given. Dr. Kovach and Dr. Abel of the Morgantown facility sent backup data, but these were not detailed enough to calculate mass balances for the trace elements. A further report is being prepared which may contain additional data to enable mass balances to be determined. Therefore, at present, no attempt has been made to distribute the trace metals between the various output waste streams. The module is set up so that coefficients can easily be added when data become available.

3.4 AFBC Module Description

The module computes the air and solid waste residuals which result from the combustion of coal in a utility AFBC boiler. Figure 3.2 gives the overall view of the module design. The module is called with the following arguments.

Total input quantity of coal
Input vector of coal characteristics
Input vector of limestone characteristics
Output vector of bottom bed material composition
Output vector of cyclone ash composition
Output vector of baghouse ash compositon
Output vector of stack gas composition
Percentage removal of SO_2
Bed height (ft)

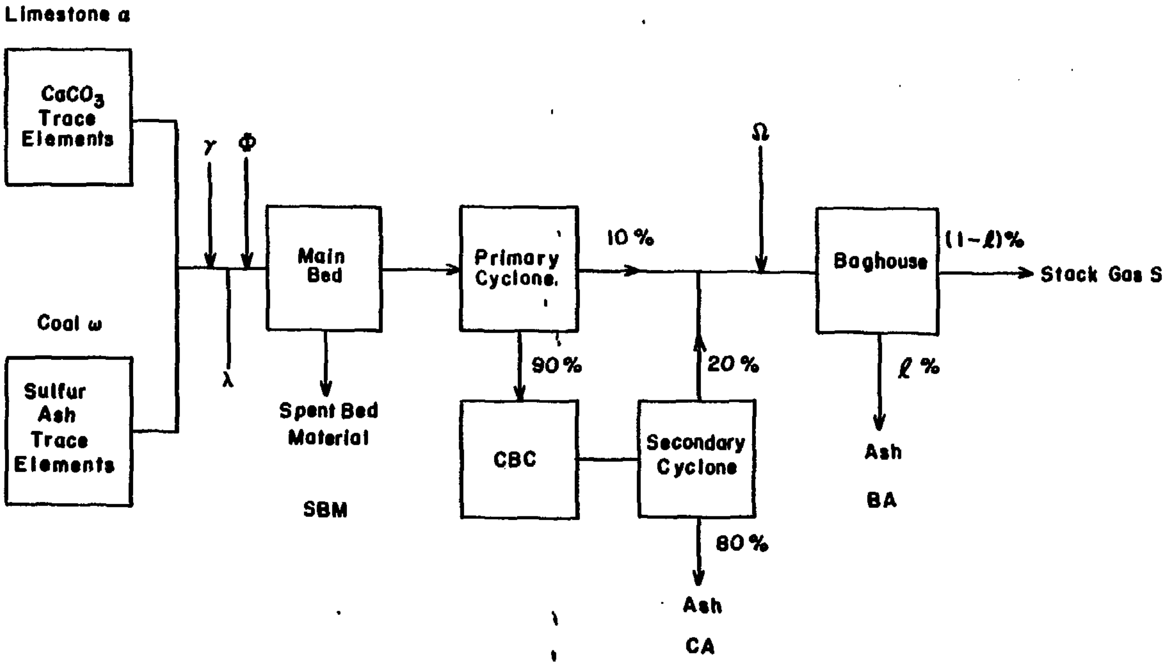

Figure 3.2 Overall AFBC Module Design

Notation for Figure 3.2

INPUTS

ω	Coal characteristics (expressed as tons)
α	Limestone characteristics (expressed as percentages)
λ	Percentage removal of SO_2
γ	Bed height (ft)
Φ	Bed velocity (ft/sec)
Ω	Allowable particulates emissions (tons/10^{12} Btu)

OUTPUTS

ℓ	Percentage removal of particulates
SBM	Amount and composition of spent bed material
CA	Amount and composition of the particulates captured by the secondary cyclone
BA	Amount and composition of the particulates captured by the baghouse
S	Composition of stack gas

Bed velocity (ft/sec)

Allowable particulate emissions (tons/10^{12} Btu input)

The input and output vectors each contain 50 elements (Table 3.1). Since these vectors are constructed to be conformable to any of the solid waste modules which have been produced, there are presently some empty elements (48 to 50, not shown in Table 3.1) and some elements not applicable to this module, which are disregarded (set to 0) in the output vectors and omitted in the output printout.

The input and output vectors give the amount of each element in tons, the exception being the input limestone vector. In this case the elements are given in terms of percentage composition because the total quantity of limestone is calculated internally in the module.

The module first calculates the Ca/S ratio using the following equation:

$$Ca/S = \frac{0.3782\ e^{2.14\eta SO_2}}{\sqrt{(H/V)}} ,$$

where

SO_2 = removal percentage SO_2,

H = bed height (ft),

V = superficial velocity (ft/sec).

From this, the total quantity of limestone required can be computed using the equation given in Table 3.2. The amount of each element in the limestone can then be computed. The $CaCO_3$ in the limestone reacts with the SO_2 according to the reactions given below.

$$CaCO_3 \longrightarrow CaO + CO_2$$

$$CaO + SO_2 + \frac{1}{} O_2 \longrightarrow CaSO_4$$

Table 3.1
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

Table 3.2
Composition of Spent Sorbent Material

Component	Equation
Limestone (Q_{LS})	$(3.125 \times S \times R)/LS_{CaCO_3}$
Calcium oxide (unreacted) (CaO)	$(0.56 \times LS_{CaCO_3} \times Q_{LS}) - (1.75 \times S \times SO_x)$
Calcium sulfate ($CaSO_4$)	$4.25 \times SO_x \times S$
Inert material (QI)	$Q_{LS} - (Q_{LS} \times LS_{CaCO_3})$

S = Input sulfur.
R = Ca/S ratio.
LS_{CaCO_3} = Percentage of $CaCO_3$ in the limestone.
SO_x = Percentage removal of SO_2.

Table 3.3
Total Solid Waste Distribution

Component	Equation
Total spent sorbent material (SBM)	$CaO + CaSO_4 + Q_I$
Bottom bed material	0.6 SBM
Cyclone	0.288 SBM + 0.72A + 0.0072C
Baghouse	(0.112 SBM + 0.28A + 0.012C) TSP

A = Input ash.
C = Input carbon.
TSP = Baghouse efficiency (see Appendix 3A for details).

The spent sorbent material therefore consists of $CaSO_4$, unreacted CaO, and inert mineral impurities in the limestone. Table 3.2 gives the equations used to calculate these components. In addition, the solid waste contains coal ash and unburnt carbon. Table 3.3 gives the equations used to calculate the total solid waste from the bottom bed drains, the secondary cyclone, and the baghous filter. The small quantity of particulate matter in the stack gas is computed by subtracting the solid waste from the three collection points from the total waste formed. A mass balance approach is then employed to distribute the elements between the bed, cyclone, baghouse, and stack gas. Table 3.4 gives the coefficients used.

The coefficients for the trace metals are at present zero. When data become available it will be a simple job to change the zeros in the data file to the new coefficients.

For sulfur, the fraction of the input amount not captured by the limestone is assumed to be converted to SO_2 and appears in the output stack gas vector under element 35. The CO_2 in the stack gas (element 42) comes from both the combustion of carbon and the conversion of $CaCO_3$ to CaO.

The appendices give further information on the source of the coefficients and details of the computer code.

Table 3.4
Coefficients for the Distribution of Elements Between Output Streams

Variable	Array Element No.	Spent Bed	Cyclone	Baghouse	Stack Gas
Ash	1	0.0	0.72	0.28 §TSP	0.28(1-§TSP)
Sulfur	2	SO_2			
Calcium sulfate	28	0.6	0.288	0.112 §TSP	0.112(1-§TSP)
Sulfur dioxide	35				$(1-SO_2)x2$
Carbon	40	0.0	0.0072	0.012 §TSP	0.012(1-§TSP)
Carbon dioxide	42				$3.6C+0.44Q_{CaCO_3}$
Calcium oxide	48	0.6	0.288	0.112 §TSP	0.112(1-§TSP)

SO_2 = Percentage removal of SO_2.
§TSP = Percentage removal of particulates.
C = Input carbon.
Q_{CaCO_3} = Input calcium carbonate.

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1. D.N. Garner, P.S. Dzierlenga and D.N. Garner, A comparison of selected design aspects of three atmospheric fluidized bed combustion conceptual power plant designs, Proc. 5th Int. Conf: Fluidized Combust., Washington, DC, 1977.

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APPENDIX 3A

CALCULATION OF MAJOR COMPONENTS OF THE SOLID WASTE

3A.1 Ca/S Molar Ratio (R)

The equation used was developed by IRµT using data from a model developed by Babcock and Wilcox in their conceptual studies of AFB boilers[2].

$$R = \frac{0.3782\ e^{2.147\eta}\ SO_x}{\sqrt{H/V}},$$

where

SO_x = removal percentage for SO_2,

H = bed height (ft),

V = superficial velocity (ft/sec).

3A.2 Amount of Limestone Required

$$\text{Input ton atoms of sulfur} = \frac{S}{\text{MW sulfur}},$$

where

S = input quantity of sulfur.

MW = molecular weight.

$$\text{Moles } CaCO_3 \text{ required} = \frac{S \times R}{\text{MW sulfur}}.$$

$$\text{Quantity of } CaCO_3 \text{ required} = \frac{S \times R \times \text{MW } CaCO_3}{\text{MW Sulfur}} \text{ tons.}$$

$$= \frac{S \times R \times 100}{32} = 3.125 \times R \times S \text{ tons.}$$

Quantity of limestone required (Q_{LS})

$$Q_{LS} = \frac{3.125 \times S \times R}{LS_{CaCO_3}} \text{ tons,}$$

where

LS_{CaCO_3} = the fraction of the limestone which is composed of $CaCO_3$.

3A.3 Spent Sorbent Material

$CaCO_3$ reacts with SO_2 according to the following equations:

$$CaCO_3 \xrightarrow{\qquad\qquad} CaO + CO_2$$

$$CaO + SO_2 + \frac{1}{2} O_2 \xrightarrow{\qquad\qquad} C_aSO_4$$

The spent sorbent material is composed of unreacted CaO, $CaSO_4$ and inert mineral matter in the limestone.

Calcium Oxide Formed (CaO_f)

$$CaO_f = Q_{CaCO_3} \times \frac{MW\ CaO}{MW\ CaCO_3}.$$

$$= Q_{CaCO_3} \times \frac{56}{100} = 0.56\ Q_{CaCO_3}.$$

Calcium Oxide Consumed During Reaction With SO_2 (CaO_c)

$$CaO_c = \frac{MW\ CaO}{MW\ sulfur} \times S \times \quad SO_x.$$

$$= \frac{56}{32} \times S \times \quad SO_x = 1.75 \times \quad SO_x.$$

Unreacted Calcium Oxide (CaO_{UR})

$$CaO_{UR} = (0.56\ Q_{CaCO_3}) - (1.75 \times S \times \quad SO_x).$$

Calcium Sulfate Formed ($CaSO_4$)

$$CaSO_4 = \frac{MW\ CaSO_4}{MW\ CaO} \times CaO_c \text{ tons}.$$

$$= \frac{136}{56} \times 1.75 \times S \times \quad SO_x\ .$$

$$= 4.25 \times S \times \quad SO_x.$$

Inert Mineral Matter (Q_I)

$Q_I = Q_{LS} - (Q_{LS} \times LS_{CaCO_3})$.

Total Spent Sorbent (SS)

$SS = CaO_{UR} + CaSO_4 + Q_I$.

3A.4 Bottom Bed Solid Waste

The module assumes that the bottom bed solid waste consists of 60% of the spent sorbent material[1,3].

Total Solid Waste = 0.60 x SS tons.

BB CaO (element 47) = 0.6 x CaO_{UR} tons.

BB $CaSO_4$ (element 28) = 0.60 x $CaSO_4$ tons.

3A.5 Solid Waste from Secondary Cyclone

The module assumes the following elutriation rates[3]:

40% of the spent sorbent material,
100% of the input ash,
10% of the input carbon.

This waste is collected in the primary cyclone where 90% is captured, the remaining 10% going to the baghouse. The captured material goes to the CBC. Here 90% of the carbon is consumed, the remaining 10% and all the input ash and spent sorbent material going to the secondary cyclone. 80% of the material into the secondary cyclone is captured and appears as solid waste, the remaining 20% goes to the baghouse.

Spent Sorbent

$$\text{Total Spent Sorbent } (C_{SS}) = 0.4 \times SS \times 0.9 \times 0.8,$$

$$= 0.288\ SS,$$

Likewise

$$C_{CaO} = 0.288\ CaO_{UR},$$

$$C_{CaSO_4} = 0.288\ CaSO_4.$$

Ash

$$C_{ASH} = ASH \times 0.9 \times 0.8 \text{ tons},$$

$$= 0.72\ ASH,$$

where

ASH = total input ash.

Carbon

Carbon into CBC = 0.1C x 0.9 tons. If 90% of carbon is consumed in the CBC, 10% goes to secondary cyclone.

$$C_{Carbon} = 0.1C \times 0.9 \times 0.1 \times 0.8,$$

$$= 0.0072C.$$

where

C = total input carbon to AFB.

Total Cyclone Solid Waste

$$C_{SW} = C_{SS} + C_{ASH} + C_{Carbon},$$

$$= 0.288_{SS} + 0.72\ ASH + 0.0072C \text{ tons}.$$

3A.6 Solid Waste from Baghouse

Total Loading for Baghouse

Spent Sorbent. The input to the baghouse is the quantity elutriated from the main bed less that captured in the secondary cyclone.

$$IB_{SS} = 0.4SS - 0.288SS,$$

$$= 0.112SS.$$

Ash. Again the input is the amount elutriated from the main bed less that captured in the secondary cyclone.

$$IB_{ASH} = ASH - 0.72\ ASH$$
$$= 0.28\ ASH.$$

Carbon. The input carbon to the baghouse is the carbon elutriated from the main bed less that captured in the cyclone, less that consumed in the CBC.

$$IB_{Carbon} = 0.1C - 0.0072C - 0.081C,$$
$$= 0.012C.$$

Total Solid Waste into Baghouse

$$IB_{SW} = 0.122SS + 0.28ASH + 0.012C.$$

Allowable Emissions from Baghouse. The allowable particulate emissions from the AFB boilers (TSP) are given as an input in terms of tons particulates/10^{12} Btu input. Also given as element 41 of the input coal characteristic vector is the total Btu value of the coal (H). From this, the total allowable emissions (E_{TSP}) for the input quantity of coal can be calculated:

$$E_{TSP} = \frac{TSP \times H}{10^{12}} .$$

The efficiency of the baghouse required to produce the allowable emissions can be calculated as follows:

$$\delta TSP = \frac{IB_{SW} - E_{TSP}}{IB_{SW}} .$$

Solid Waste from Baghouse. This is given simply as the input to the baghouse multiplied by the efficiency of the baghouse.

$$B_{SW} = IB_{SW} \times \delta \text{ TSP},$$

$$B_{CaO} = 0.112 \text{ CaO}_{UR} \times \delta \text{ TSP},$$

$$B_{CaSO_4} = 0.112 \text{ CaSO}_4 \times \delta \text{ TSP},$$

$$B_{ASH} = 0.28 \text{ ASH} \times \delta \text{ TSP tons},$$

$$B_{Carbon} = 0.012C \times \delta \text{ TSP tons}.$$

3A.7 Carbon Dioxide Produced

CO_2 from Carbon Combustion. Carbon is combusted to form CO_2 in the main bed and CBC. The module assumes 90% combustion in the main bed. The remaining 10% goes to the primary cyclone where 90% is captured and sent to the CBC, where a further 90% is combusted[3].

$$C_{CO_2} = \frac{\text{MW } CO_2}{\text{MW carbon}} \;(0.9C + (0.1C \times 0.9 \times 0.9)),$$

$$= \frac{44}{12} \;(0.9C + 0.081C),$$

$$= 3.6C \text{ tons}.$$

CO_2 from Limestone. When limestone reacts with SO_2, CO_2 is formed (see equations in Section 3A.3):

$$LS_{CO_2} = Q_{CaCO_3} \times \frac{\text{MW } CO_2}{\text{MW } CaCO_3},$$

$$= Q_{CaCO_3} \times \frac{44}{100} = 0.44\, Q_{CaCO_3}.$$

Total CO_2 Produced

$$CO_2 = 3.60C + 0.44\, Q_{CaCO_3}.$$

3A.8 SO_2 Produced

Captured sulfur (CS) = S x δ SO_2.

$$SO_2 = (S - CS) \times \frac{\text{MW } SO_2}{\text{MW sulfur}}$$

$$= (S - (S \times \delta\ SO_2) \times \frac{64}{32},$$

$$= 2S\ (1 - \delta\ SO_2) \text{ tons.}$$

APPENDIX 3B

DESCRIPTION OF COMPUTER MODULE

The AFBC solid waste module consists of one subroutine and a data file containing the fraction of the input components that are removed to the different output streams. The module is set in motion by a call to AFBC:

CALL AFBC (Q, COAL, LIMEST, BED, CYCL, BAG, STACK, SO2EFF, BEDHT, BEDV,
TSPEM),

where

Q = total mass of input coal

COAL = input coal characteristic vector

LIMEST = input limestone characteristic vector

BED = bottom bed waste output characteristic vector

CYCL = cyclone waste output characteristic vector

BAG = baghouse waste output characteristic vector

STACK = stack gas output characteristic vector

SO2EFF = percentage removal of SO_2

BEDHT = bed height (ft)

BEDV = bed velocity (ft/sec)

TSPEM = allowable particulate emissions (tons/10^{12} Btu)

The subroutine first reads the removal coefficients from file "TAPE1". Thereafter, if the amounts of radium-226, radium-228, and lead-210 are zero in the coal input vector, the quantities are calculated based on uranium-238 and thorium-232 (see Section 7).

The total amount of limestone (QLS) required in the AFB process is then computed as a function of the Ca/S ratio (CASRAT), sulfur removal efficiency

(SO2EFF), the bed height and velocity (BEDHT, BEDV), and the amount of sulfur in the input coal (see Appendix 3A). From this amount the total spent bed material (SBM) is calculated from its estimated components: calcium oxide (CAO), calcium sulfate (CASO4) and total inert materials (QI). The amounts of the individual components are then calculated by multiplying QLS by the fraction of each of the components of the input limestone (the original entries of the input limestone vector). These quantities replace the fractions in the limestone vector. (As before, if the radium and lead entries are zero, they are calculated as in Section 7.)

The total amounts of solid waste from the bed, cyclone and baghouse are then calculated as described in Appendix 3A.

A "DO" loop then multiplies the removal coefficients by the input coal vector to obtain the amount of each component which is contained in each of the solid waste output vectors. As mentioned previously, there are presently no data for trace metal removal, and consequently all coefficients for these are zero.

Special Calculations Not Performed in "DO" Loop

1. Total solid waste (output array element 25 (AE25)) for each of the vectors was calculated previously and is therefore bypassed in the "DO" loop.

2. Certain elements are affected by the TSP removal efficiency (NTSP) which is calculated in the program to estimate total solid waste from the baghouse. These elements must be multiplied by NTSP (or 1-NTSP) after having been multiplied by the removal coefficients. These elements are ash (AE1), carbon (AE40), and calcium sulfate and oxide (AE28 and AE47 - see below).

3. The amount of sulfur in the bottom bed waste is a function of the SO_2 efficiency. This is calculated by multiplying input sulfur by SO2EFF.

4. The output quantities of calcium sulfate and calcium oxide are a function of the amounts of each, respectively, that are in the input limestone. The output quantities are calculated by multiplying the respective removal rates by $CASO_4$ and CAO. The amounts removed by the baghouse, which are a function of NTSP, are calculated accordingly (see 2, above).

5. The amount of carbon dioxide (AE42) which goes up the stack is a function of the input carbon in the coal and the calcium carbonate in the limestone, and is calculated as discussed in Appendix 3A.

APPENDIX 3C

COMPUTER CODE AND SAMPLE OUTPUT

This section gives the computer code used for the AFBC module and the data file of coefficients, with a sample input and the resulting output. Tables 3C.1 and 3C.2 give the coal and limestone characteristics used as input. The other input variables are as follows:

Quantity of coal (Q) = 100,000.0 tons.

SO_2 removal (SO2EFF) = 85.0%

Bed height (BEDHT) = 3 ft.

Bed velocity (BEDV) = 12 ft/sec

Particulate emissions (TSPEM) = 15 tons/10^{12} Btu input.

The main program of the code is used only to set the input variables.

Table 3C.1
Input Coal Characteristics

Element	Input Quantity (tons)	Element	Input Quantity (tons)
Ash	9200.0	Manganese	20.0
Sulfur	2500.0	Mercury	0.014
Antimony	0.08	Nickel	1.5
Arsenic	1.1	Selenium	0.35
Beryllium	0.2	Silver	0.02
Cadmium	0.03	Thallium	0.02
Chromium	1.5	Zinc	1.28
Copper	1.6	Uranium	0.1
Iron	1000.0	Thorium	0.28
Lead	1.09	Pyritic sulfur	1870.0
Magnesium	52.0	Carbon	64100.0
		Btu	$2.3x10^{12}$

Table 3C.2
Input Limestone Characteristics

Element	Fractional Composition	Element	Fractional Composition
Ash	0.0	Magnesium	0.01
Sulfur	0.0	Manganese	60.0×10^{-6}
Antimony	0.3×10^{-6}	Mercury	0.0
Arsenic	6.0×10^{-6}	Nickel	6.0×10^{-6}
Beryllium	2.0×10^{-6}	Selenium	3.0×10^{-6}
Cadmium	0.3×10^{-6}	Silver	0.1×10^{-6}
Chromium	20.0×10^{-6}	Thallium	0.1×10^{-6}
Copper	2.0×10^{-6}	Zinc	30.0×10^{-6}
Iron	1.0×10^{-3}	Uranium	2.7×10^{-6}
Lead	3.0×10^{-6}	Thorium	3.4×10^{-6}
		Calcium carbonate	0.90

```
      PROGRAM FLUID(OUTPUT,TAPE1,TAPE2=OUTPUT)
      DIMENSION COAL(50),BED(50),CYCL(50),BAG(50),STACK(50)
      REAL LIMEST(50)
            Q=100000.00
            SO2EFF=85.
            BEDHT=3.
            BEDV=12.
            TSPEM=15.
            COAL(1)=9200.
            COAL(2)=2500.
            COAL(3)=0.08
            COAL(4)=1.1
            COAL(5)=0.2
            COAL(6)=0.03
            COAL(7)=1.5
            COAL(8)=1.6
            COAL(9)=1000.0
            COAL(10)=1.09
            COAL(11)=52.0
            COAL(12)=20.0
            COAL(13)=0.014
            COAL(14)=1.5
            COAL(15)=0.35
            COAL(16)=0.02
            COAL(17)=0.02
            COAL(18)=1.28
            COAL(19)=0.1
            COAL(20)=0.28
            DO 10 I=21,38
            COAL(I)=0.
10 CONTINUE
            COAL(39)=1870
            COAL(40)=64100
            COAL(41)=2.3E12
            DO 20 I=42,50
            COAL(I)=0.
20 CONTINUE
            LIMEST(1)=0.
            LIMEST(2)=0.
            LIMEST(3)=0.3E-6
            LIMEST(4)=6.E-6
            LIMEST(5)=2.E-6
            LIMEST(6)=.3E-6
            LIMEST(7)=20.E-6
            LIMEST(8)=2.E-6
            LIMEST(9)=1.E-3
            LIMEST(10)=3.E-6
            LIMEST(11)=0.01
            LIMEST(12)=60.E-6
            LIMEST(13)=0.0
            LIMEST(14)=6.E-6
```

```
          LIMEST(15)=3.E-6
          LIMEST(16)=0.1E-6
          LIMEST(17)=0.1E-6
          LIMEST(18)=30.E-6
          LIMEST(19)=2.7E-6
          LIMEST(20)=3.4E-6
          DO 30 I=21,45
          LIMEST(I)=0.
  30  CONTINUE
          LIMEST(46)=.9
          DO 40 I=47,50
          LIMEST(I)=0.
  40  CONTINUE
          CALL AFBC(Q,COAL,LIMEST,BED,CYCL,BAG,STACK,SO2EFF,BEDHT,
     -BEDV,TSPEM)
      STOP
      END



      SUBROUTINE AFBC(Q,COAL,LIMEST,BED,CYCL,BAG,STACK,SO2EFF,BEDHT,
     -BEDV,TSPEM)
      DIMENSION COAL(50),BED(50),CYCL(50),BAG(50),STACK(50),
     -BEDC(50),CYCLC(50),BAGC(50),STACKC(50)
      REAL LIMEST(50),NTSP,IBSW
C   * REMOVAL COEFFICIENTS READ IN FROM DATA FILE *
      READ(1,1000)(BEDC(I),CYCLC(I),BAGC(I),STACKC(I),I=1,50)
C   * CALCULATION OF RA-226,RA-228 &PB-210 IN COAL IF NOT GIVEN AS INPUT
      IF(COAL(21) .EQ. 0.)COAL(21)=3.38E-7*COAL(19)
      IF(COAL(22) .EQ. 0.)COAL(22)=4.01E-10*COAL(20)
      IF(COAL(23) .EQ. 0.)COAL(23)=4.37E-9*COAL(19)
1000  FORMAT(4F10.5)
      SO2EFF=SO2EFF/100.
C   * CALCULATION OF CA/S MOLAR RATIO
      CASRAT=.3782*EXP(2.14*SO2EFF)/SQRT(BEDHT/BEDV)
C   * CALCULATION OF QUANTITY OF LIMESTONE REQUIRED
      QLS=3.125*COAL(2)*CASRAT/LIMEST(46)
C   * CALCULATION OF CAO,CASO4 AND INERT MATERIAL IN SPENT BED MATERIAL
      CAO=.56*LIMEST(46)*QLS-1.75*COAL(2)*SO2EFF
      CASO4=4.25*COAL(2)*SO2EFF
      QI=QLS-QLS*LIMEST(46)
C   * CALCULATION OF TOTAL SPENT BED MATERIAL
      SBM=CAO+CASO4+QI
C   * QUANTITIES OF INPUT ELEMENTS IN LIMESTONE CALCULATED
      DO 10 I=1,50
      LIMEST(I)=QLS*LIMEST(I)
   10 CONTINUE
C   * CALCULATION OF RA-226,RA-228 & PB-210 IN LIMESTONE
      IF(LIMEST(21).EQ.0.)LIMEST(21)=3.38E-7*LIMEST(19)
      IF(LIMEST(22).EQ.0.)LIMEST(22)=4.0E-10*LIMEST(20)
      IF(LIMEST(23).EQ.0.)LIMEST(23)=4.37E-9*LIMEST(19)
C   * CALCULATION OF TOTAL BOTTOM BED MATERIAL
      BED(25)=.6*SBM
C   * CALCULATION OF TOTAL CYCLONE SOLID WASTE
      CYCL(25)=.288*SBM+.72*COAL(1)+.0072*COAL(40)
C   * CALCULATION OF ALLOWABLE TSP EMISSIONS
      ETSP=TSPEM*COAL(41)/1.E12
C   * CALCULATION OF INPUT LOADING TO BAGHOUSE
      IBSW=.112*SBM+.28*COAL(1)+.012*COAL(40)
```

```
C   * CALCULATION OF REQUIRED BAGHOUSE EFFICICENCY
      NTSP=(IBSW-ETSP)/IBSW
C   * CALCULATION OF TOTAL BAGHOUSE SOLID WASTE
      BAG(25)=(.112*SBM+.28*COAL(1)+.012*COAL(40))*NTSP
C   * CALCULATION OF QUANTITY OF EACH ELEMENT IN EACH WASTE STREAM
      DO 20 I=1,50
C   * I=25 IS THE TOTAL SOLID WASTE WHICH HAS ALREADY BEEN CALCULATED
      IF(I .EQ. 25)GO TO 20
      BED(I)=COAL(I)*BEDC(I)
      CYCL(I)=COAL(I)*CYCLC(I)
      BAG(I)=COAL(I)*BAGC(I)
      STACK(I)=COAL(I)*STACKC(I)
   20 CONTINUE
      STACK(25)=0.
C   * CALCULATION OF AMOUNT OF TSP IN BAGHOUSE AND STACK GAS
      BAG(1)=BAG(1)*NTSP
      STACK(1)=STACK(1)*(1.-NTSP)
C   * CALCULATION OF AMOUNT OF SULFUR IN BOTTOM BED MATERIAL
      BED(2)=COAL(2)*SO2EFF
C   * CALCULATION OG THE AMOUNT OF CASO4 IN EACH WASTE STREAM
      BED(28)=CASO4*BEDC(28)
      CYCL(28)=CASO4*CYCLC(28)
      BAG(28)=CASO4*BAGC(28)*NTSP
      STACK(28)=CASO4*STACKC(28)*(1.-NTSP)
C   * CALCULATION OF AMOUNT OF SO2 IN STACK GAS
      STACK(35)=COAL(2)*2*(1.-SO2EFF)
C   * CALCULATION OF AMOUNT OF CARBON IN BAGHOUSE AND STACK GAS
      BAG(40)=BAG(40)*NTSP
      STACK(40)=STACK(40)*(1.-NTSP)
C   * CALCULATION OF AMOUNT OF CO2 IN STACK GAS
      STACK(42)=3.6*COAL(40)+.44*LIMEST(46)
C   * CALCULATION OF AMOUNT OF CAO IN EACH WASTE STREAM
      BED(47)=CAO*BEDC(47)
      CYCL(47)=CAO*CYCLC(47)
      BAG(47)=CAO*BAGC(47)*NTSP
      STACK(47)=CAO*STACKC(47)*(1.-NTSP)
      WRITE(2,100)
  100 FORMAT(1H1)
      WRITE(2,2000)Q,QLS,(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),
     -STACK(I),I=1,4)
 2000 FORMAT(1X,*TOTAL INPUT COAL:*,T31,E12.5/1X,*TOTAL LIMESTONE REQUIR
     -ED:*,T31,E12.5//1X,*ELEMENT*,T21,*INPUT COAL*,T36,*LIMESTONE*,T51,
     -*SPENT BED MAT.*,T66,*CYCLONE*,T81,*BAGHOUSE*,T96,*STACK*/
     -1X,106(*-*)/1X,*ASH*,T20,E12.5,5(3X,E12.5)/
     -1X,*SULFUR*,T20,E12.5,5(3X,E12.5)/
     -1X,*ANTIMONY*,T20,E12.5,5(3X,E12.5)/
     -1X,*ARSENIC*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2001)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),
     -I=5,8)
 2001 FORMAT(1X,*BERYLLIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*CADMIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*CHROMIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*COPPER*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2002)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),
     -I=9,12)
```

```
2002 FORMAT(1X,*IRON*,T20,E12.5,5(3X,E12.5)/
     -1X,*LEAD*,T20,E12.5,5(3X,E12.5)/
     -1X,*MAGNESIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*MANGANESE*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2003)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),
     -I=13,16)
2003 FORMAT(1X,*MERCURY*,T20,E12.5,5(3X,E12.5)/
     -1X,*NICKEL*,T20,E12.5,5(3X,E12.5)/
     -1X,*SELENIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*SILVER*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2004)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),
     -I=17,20)
2004 FORMAT(1X,*THALLIUM*,T20,E12.5,5(3X,E12.5)/
     -1X,*ZINC*,T20,E12.5,5(3X,E12.5)/
     -1X,*URANIUM-238*,T20,E12.5,5(3X,E12.5)/
     -1X,*THORIUM-232*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2005)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),
     -I=21,23),
     -COAL(25),LIMEST(25),BED(25),CYCL(25),BAG(25),STACK(25),
     -COAL(28),LIMEST(28),BED(28),CYCL(28),BAG(28),STACK(28)
2005 FORMAT(1X,*RADIUM-226*,T20,E12.5,5(3X,E12.5)/
     -1X,*RADIUM-228*,T20,E12.5,5(3X,E12.5)/
     -1X,*LEAD-210*,T20,E12.5,5(3X,E12.5)/
     -1X,*TOTAL SOLID WASTE*,T20,E12.5,5(3X,E12.5)/
     -1X,*CALCIUM SULFATE*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2006)COAL(35),LIMEST(35),BED(35),CYCL(35),BAG(35),
     -STACK(35),
     -(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),STACK(I),I=40,42)
2006 FORMAT(1X,*SULFUR DIOXIDE*,T20,E12.5,5(3X,E12.5)/
     -1X,*CARBON*,T20,E12.5,5(3X,E12.5)/
     -1X,*BTU*,T20,E12.5,5(3X,E12.5)/
     -1X,*CARBON DIOXIDE*,T20,E12.5,5(3X,E12.5))
      WRITE(2,2007)(COAL(I),LIMEST(I),BED(I),CYCL(I),BAG(I),
     -STACK(I),I=46,47)
2007 FORMAT(1X,*CALCIUM CARBONATE*,T20,E12.5,5(3X,E12.5)/
     -1X,*CALCIUM OXIDE*,T20,E12.5,5(3X,E12.5))
      RETURN
      END
```

```
 0.          .72        .28        .28
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
 0.          0.         0.         0.
.6          .288       .112       .112
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         2.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          .0072      .012       .012
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
.6          .288       .112       .112
0.          0.         0.         0.
0.          0.         0.         0.
0.          0.         0.         0.
```

```
TOTAL INPUT COAL:              .10000E+06
TOTAL LIMESTONE REQUIRED:      .40484E+05

ELEMENT            INPUT COAL     LIMESTONE    SPENT BED MAT. CYCLONE      BAGHOUSE       STACK
-------------------------------------------------------------------------------------------------------
ASH                 .92000E+04    0.           0.              .66240E+04    .25627E+04    .13306E+02
SULFUR              .25000E+04    0.            .21250E+04    0.           0.             0.
ANTIMONY            .80000E-01     .12145E-01  0.             0.           0.             0.
ARSENIC             .11000E+01     .24290E+00  0.             0.           0.             0.
BERYLLIUM           .20000E+00     .80967E-01  0.             0.           0.             0.
CADMIUM             .30000E-01     .12145E-01  0.             0.           0.             0.
CHROMIUM            .15000E+01     .80967E+00  0.             0.           0.             0.
COPPER              .16000E+01     .80967E-01  0.             0.           0.             0.
IRON                .10000E+04     .40484E+02  0.             0.           0.             0.
LEAD                .10900E+01     .12145E+00  0.             0.           0.             0.
MAGNESIUM           .52000E+02     .40484E+03  0.             0.           0.             0.
MANGANESE           .20000E+02     .24290E+01  0.             0.           0.             0.
MERCURY             .14000E-01    0.           0.             0.           0.             0.
NICKEL              .15000E+01     .24290E+00  0.             0.           0.             0.
SELENIUM            .35000E+00     .12145E+00  0.             0.           0.             0.
SILVER              .20000E-01     .40484E-02  0.             0.           0.             0.
THALLIUM            .20000E-01     .40484E-02  0.             0.           0.             0.
ZINC                .12800E+01     .12145E+01  0.             0.           0.             0.
URANIUM-238         .10000E+00     .10931E+00  0.             0.           0.             0.
THORIUM-232         .28000E+00     .13764E+00  0.             0.           0.             0.
RADIUM-226          .33800E-07     .36945E-07  0.             0.           0.             0.
RADIUM-228          .11228E-09     .55058E-10  0.             0.           0.             0.
LEAD-210            .43700E-09     .47767E-09  0.             0.           0.             0.
TOTAL SOLID WASTE  0.             0.            .17859E+05     .15658E+05    .66443E+04   0.
CALCIUM SULFATE    0.             0.            .54188E+04     .26010E+04    .10063E+04    .52250E+01
SULFUR DIOXIDE     0.             0.           0.             0.           0.             .75000E+03
CARBON              .64100E+05    0.           0.              .46152E+03    .76523E+03    .39734E+01
BTU                 .23000E+13    0.           0.             0.           0.             0.
CARBON DIOXIDE     0.             0.           0.             0.           0.             .24679E+06
CALCIUM CARBONATE  0.             .36435E+05  0.             0.           0.             0.
CALCIUM OXIDE      0.             0.            .10011E+05     .48053E+04    .18591E+04    .96530E+01
```

4. SOLID WASTE MODULE FOR LURGI PROCESS COAL GASIFICATION

4.1. Introduction

Increased demand for liquid and gaseous fuels, coupled with decreasing domestic supply, has led to an increasing interest in the synthetic production of fuel oils and gases from coal. The coal supplies of the U.S. are sufficiently abundant to supply the country with energy for decades. While many existing large facilities could convert directly from oil and natural gas to coal, other fuel-consuming activities, e.g., residential heating, could not change over to coal without enormous costs in modification of present equipment and addition of pollution control devices to prevent adverse environmental effects. Production of synthetic fuels from coal would, in effect, eliminate the need to modify existing equipment. In particular, coal gasification is capable of creating a high Btu synthetic natural gas (SNG) which can be used as a direct substitute for natural gas and as such can use existing storage and transportation facilities (pipelines and rail and truck distribution systems). Low and medium Btu gas can also be produced from coal.

4.1.1 Lurgi Gasifiers

Techniques for coal gasification have been in existence for many years. Modern techniques of gasification had their origin in Germany, and the first commercial coal gasifier was built in Hirschfelde, Germany, in 1936. The process used in this first plant is known as the Lurgi process. While there are other types of gasifiers (e.g., Synthane, Hygas, etc.), most commercial gasification plants are Lurgi. To date, there are eighteen foreign low and medium Btu commercial Lurgi gasification facilities. There are five commercial low Btu gasifiers in the U.S. that are in production or near completion. While there are no commercial high Btu gasifiers in existence, there are several ongoing DOE-sponsored demonstration projects.

All solid waste estimates in this module are based on Lurgi gasifier data. While there is no reason to believe that the solid waste streams from all types of gasification will be similar in composition to that generated by the Lurgi process, use of Lurgi data as a basis for estimation is an acceptable compromise in determining the composition of solid waste for several reasons:

- very little data on solid waste are available for other types of gasification;
- solid waste from some other processes (e.g., ash from the Synthane process) is not expected to be significantly different from Lurgi[1] (although Synthane produces little or no tar and oil condensates as does Lurgi);
- since Lurgi gasifiers are already used commercially it is reasonable to assume that many new commercial gasifiers will also be Lurgi;
- present solid waste data for Lurgi are so variable that the "noise" from errors in the data may cover any difference between gasifier types.

While most of the basic processes described below pertain to all types of gasifiers, the discussion will center around the Lurgi dry ash process. Only low and high Btu gas production processes will be considered, although solid waste generation will be the same for all types (see Section 4.3).

4.2 Gasification Principles

In general, the actual gasification of coal consists of three basic steps: coal preparation, coal gasification, and gas purification. For SNG production, there is a fourth step, gas upgrading. In addition to the actual conversion of coal to gas, the following supportive (utility and pollution control) processes may be required: steam and power generation, air pollution control, water treatment, and sulfur recovery. Figure 4.1 gives a flow diagram of a "typical" Lurgi gasifier for both low Btu gas and SNG.

4.2.1 Coal Preparation

Preparation. For Lurgi applications, preparation of coal is very seldom more than breaking and sizing the coal to the .32 to 3.5-cm-diameter size necessary for the feed stream. Except for coal with a high moisture content (>36%), drying and pretreatment to prevent caking are unnecessary.

Solid Waste from Coal Preparation. Solid waste from drying and pretreatment of coal is not considered here, as these processes are rarely used. Waste from breaking and sizing is considered elsewhere (Section 1) and can be estimated using the solid waste module for physical coal cleaning.

4.2.2 Coal Gasification

Gasification. Coal is fed in through the top of the gasifier. It passes through four zones of increasing temperature in the gasification chamber before what remains exits through the bottom as ash. The four zones are, in order of entry, drying, devolatilization, gasification, and combustion. The product gas rises, counter to the coal feed, and exits near

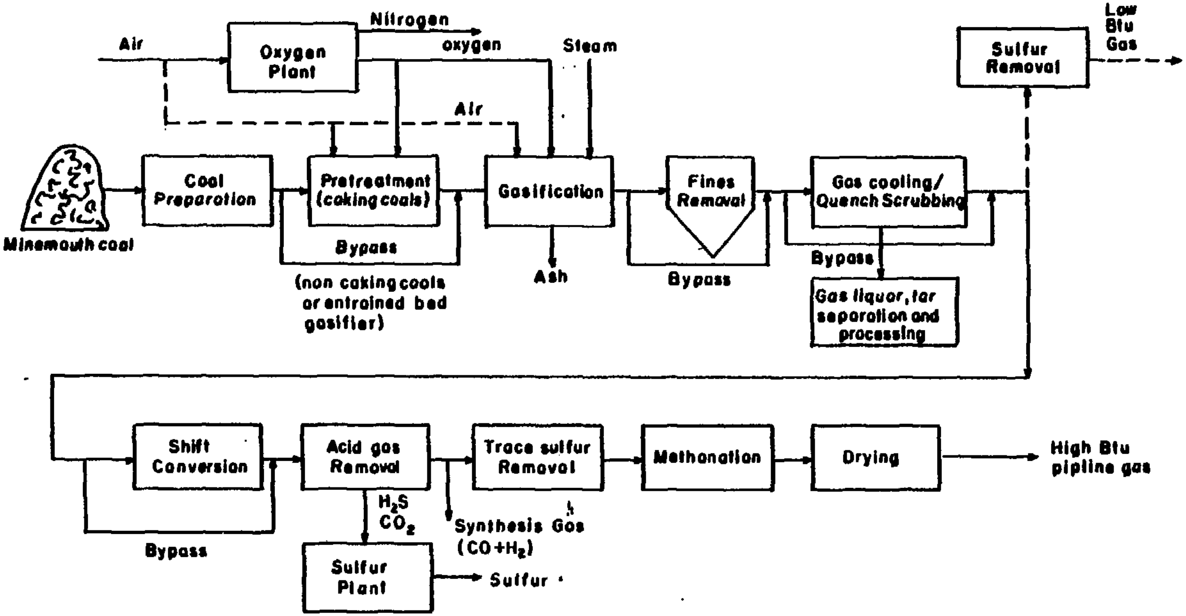

Figure 4.1 Schematic Flow Diagram of a Coal Gasification Plant (From Reference 8)

the top of the gasifier. The ash is discharged to an ash lockhopper through the bottom of the gasifier.

Solid Waste from Gasification. Solid waste from the gasification process consists of bottom ash, including some carbon, sulfur, and trace elements, along with quench water used to facilitate handling of the hot ash.

It is recognized that most of the ash and nonvolatile trace elements in the input coal are captured in the bottom ash. Highly volatile trace components (e.g., mercury, selenium, and arsenic) escape in large part with the raw product gas[2,3].

4.2.3 Gas Purification

Gas Purification Processes

Gas Cooling. Cooling the product gas after it leaves the gasification chamber results in the removal of condensable components of the raw gas and temperature reduction of the gas for further processing (in the case of SNG production). The gas is first put through a primary cooler. For production of SNG, some of this cooled gas is sent to shift reaction (see Section 4.2.4) and all of the gas is put through a secondary cooling process. As the gas cools, moisture, tars, oils, and other components of the raw gas condense and are channeled into a gas liquor stream.

Acid Gas Removal (SNG Production). For SNG production, the cooled gas must be purified of hydrogen sulfide and sulfur trace compounds. Carbon dioxide must also be removed to increase the heating value of the product gas. Lurgi systems use the Rectisol process to remove acid gas. This process is based on the absorption of CO_2, H_2S, and other compounds in cold methanol.

The acid gas is then usually sent through a sulfur recovery process to produce marketable sulfur.

Methanation Guards (SNG Production). Further removal of trace sulfur compounds is sometimes necessary to prevent contamination of the methanation catalyst (see Section 4.2.4). Methanation guards are fixed beds of adsorbents over which the product gas passes after acid gas removal. The methanation guard beds are generally of four types:

1) metal (zinc, iron or nickel) oxide
2) metal oxide - impregnated activated carbon
3) activated carbon
4) molecular sieve

Solid Waste from Gas Purification

Solid waste from gas purification falls into three basic categories: gas liquor (including separated tar and oil), recovered sulfur, and spent catalyst.

Gas Liquor from Cooling. After primary and secondary cooling, the resulting gas liquor streams are sent through tar/oil separation processes. The three output solid waste streams from these processes (separated gas liquor, tar, and oil) will contain virtually all of the remaining inorganic trace elements (except for some of the more volatile elements - see Section 4.3). They will also contain some of the noncombusted carbon and sulfur.

Solid Waste from Acid Gas Removal. Solid waste from the removal of acid gas will result only from the sulfur recovery process.

Catalysts from Methanation Guard. The methanation guard contributes to solid waste generally only in spent sorbent material. The periodicity of purging or removal of the sorbent material is not yet completely known, although time estimates of catalyst removal are from 6 months to two years[4]. Trace element constituents of the material contributed by the product gas are believed to be small enough to be disregarded. Constituents of the sorbent material itself may contribute significant concentrations of trace elements to solid waste.

4.2.4 Gas Upgrading (SNG Production). Gas upgrading consists of shift conversion of some of the (primary) cooled gas before secondary cooling, and methanation and drying of the product gas after acid gas and trace sulfur removal.

Gas Upgrading Processes

Shift Conversion. While a large part of the methane is produced in the gasification chamber, conversion of product gas to SNG which is pipeline quality requires conversion of hydrogen and carbon monoxide to methane. This in turn requires that, prior to methanation (see below), the raw gas have a 3:1 H_2/CO ratio. After primary cooling of the gasifier exit gas, some of the cooled gas (usually about 50%) is sent to shift conversion to achieve this ratio. The shift converter is usually a cobalt molybdate-based catalyst through which the gas flows.

Methanation and Drying. Methanation and drying are the final steps in producing SNG. Methanation is the catalytic reaction of carbon oxides and hydrogen to form methane and water. A nickel-based catalyst is usually used.

Drying is accomplished by condensation (for removal of most of the moisture created in methanation) and sorption (for residual moisture removal).

Solid Wastes from Gas Upgrading

Solid wastes from gas upgrading consist of the spent catalysts involved. Although data are limited, contributions of trace elements from the gas are thought to be negligible, since almost all trace elements are removed in gasifier bottom ash and gas liquor streams (see Sections 4.2.2 and 4.2.3). Contributions from the spent catalysts may be significant, although catalyst life for the methanation process is estimated to be 2 to 5 years[1].

4.2.5 Supportive Processes in Coal Gasification. Supportive processes to the gasification of coal include steam and power generation, air pollution control, water treatment, and sulfur recovery.

Supportive Processes

Steam and Power Generation. Most gasification facilities will have on-site plants for generating the steam and power needed for gasification. Fuels for this facility can include gas, oil, coal, and gasification by-products.

Air Pollution Control. Air pollution control devices, for control of emissions from gasification and supportive processes, will generally be similar to those found in conventional utility boilers, such as electrostatic precipitators and FGD systems.

Water Treatment. Water treatment processes include treatment of separated gas liquor and ash quench water.

Sulfur Recovery. Marketable sulfur can be recovered from removed acid gas.

Solid Waste from Supportive Processes

Solid waste from supportive processes generally consists only of ash from power generation, ash and sludge from air pollution control, and recovered sulfur. Wastes from power generation and air pollution control devices have been described elsewhere (Section 2); the recovered sulfur can be assumed to be almost pure (although some trace compounds may exist[5]) and can be marketed, even though here it is characterized as a waste product.

4.3. Modeling Assumptions

As mentioned before, data on solid waste, especially the trace constituents of that waste, are few and variable. Most data relate to Lurgi gasifiers and as such this module assumes the shape of a "typical" Lurgi gasifier.

Almost all data on gasifier wastes are limited to four waste streams: bottom ash, oil, tar, and separated gas liquor. No data were found on any trace elements in either recovered sulfur or spent catalysts. Since it is recognized that virtually all inorganic trace metals, ash, and noncombusted free carbon have been removed from the coal and gas by the gasification and cooling steps, it was decided to assume that all trace elements (except mercury and selenium) were found in these waste streams. Some mercury and most of the selenium are unaccounted for and are assumed to have been lost in fugitive gas emissions. Recovered sulfur is assumed to be pure sulfur with no trace contamination.

Since catalysts involved in the gasification procedures are removed or purged intermittently and their constituency is unknown, it was decided to disregard them as components of solid waste. This decision is also warranted by the fact that many of the catalysts can be recycled[1]. Inclusion of these in the module when and if data become available would be a simple task.

Solid wastes from coal preparation, power generation, and air pollution control have been characterized in other solid waste modules (Sections 1, 2); these wastes can be estimated, if necessary, by the appropriate solid waste module (or subroutine).

Because of the variability of the data, it was impossible to obtain estimates of trace element removal rates which would be a function of some characteristic of the input coal (such as trace element content). Therefore each process was assumed to remove a fixed percentage of the total mass of the input coal content of an element, for each element. These percentages are given in the next section.

The Lurgi process can produce low, medium, or high Btu product gas, the only differences being more gas purification and upgrading steps as one increases the Btu content. Production of all grades of gas include the gasification and cooling steps; since these are the only steps assumed to produce solid waste, solid wastes for all gas grades can be characterized by the module.

4.4. Coal Gasification Module Description

4.4.1 General Description

The gasification module assumes constant removal rates for each of the input elements in each of the processes which are assumed to generate all of the solid waste. The module is called with the following arguments:

- total mass of coal
- input coal characteristics vector
- output solid waste characteristics vectors

The input and output vectors each contain 50 elements. These elements are shown in Table 4.1. Since these vectors are constructed to be conformable to any of the solid waste modules which have been produced, there are presently some empty elements (48 to 50, not shown in Table 4.1) and some elements which are not applicable to this module, and as such are disregarded (set to 0) in the output vectors and omitted in the output printout.

Table 4.2 gives the coefficients which determine the amount of each element that goes to each solid waste stream. Note that most of the elements' coefficients sum to 1, reflecting the assumption of total removal in these streams. Table 4.3 gives the calculation of water and total waste for each stream. It should be noted here that, given the data, some of these coefficients are little more than conjecture as to the "true" removal rates. Future acquisition of more and better data is definitely indicated.

The appendices show how the choice of coefficients was made and give more information on the computer module.

Table 4.1
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

Table 4.2
Fractions (Coefficients) of Array Elements Going to Solid Waste Streams

Variable	Array Element No.	Bottom Ash	Oil	Tar	Gas Liquor	Sulfur Recovery	Unaccounted for
Ash	1	0.9924	0.0025	0.005	0.0001	0.0	0.0
Total sulfur	2	0.0025	0.005	0.015	0.0001	0.96	0.0174
Antimony	3	0.50	0.01	0.04	0.45	0.0	0.0
Arsenic	4	0.45	0.05	0.05	0.45	0.0	0.0
Beryllium	5	0.93	0.01	0.03	0.03	0.0	0.0
Cadmium	6	0.59	0.03	0.03	0.35	0.0	0.0
Chromium	7	0.93	0.01	0.05	0.01	0.0	0.0
Copper	8	0.96	0.01	0.02	0.01	0.0	0.0
Iron	9	0.98	0.0005	0.019	0.0005	0.0	0.0
Lead	10	0.87	0.01	0.11	0.01	0.0	0.0
Magnesium	11	0.98	0.0005	0.019	0.0005	0.0	0.0
Manganese	12	0.98	0.001	0.016	0.003	0.0	0.0
Mercury	13	0.03	0.05	0.55	0.35	0.0	0.02
Nickel	14	0.95	0.01	0.03	0.01	0.0	0.0
Selenium	15	0.10	0.01	0.01	0.01	0.0	0.87
Silver	16	0.97	0.01	0.01	0.01	0.0	0.0
Thallium	17	0.98	0.005	0.01	0.005	0.0	0.0
Zinc	18	0.91	0.02	0.04	0.03	0.0	0.0
Uranium-238	19	0.80	0.03	0.10	0.07	0.0	0.0
Thorium-232	20	0.80	0.03	0.10	0.07	0.0	0.0
Radium-226	21	0.80	0.03	0.10	0.07	0.0	0.0
Radium-228	22	0.80	0.03	0.10	0.07	0.0	0.0
Lead-210	23	0.87	0.01	0.11	0.01	0.0	0.0
Total solid waste	25		See Appendix 4A and Table 4.3				
Water	34						
Pyritic sulfur	39	0.0025	0.005	0.015	0.0001	0.96	0.0174
Carbon	40	0.008	0.01	0.03	0.0001	0.0	0.0

Table 4.3
Estimation of Water and Total
Solid Waste

Waste Stream	Water	Total Waste
Bottom ash	0.20 (ash + carbon + sulfur)	Ash + carbon + sulfur + water
Oil	0.12 (total waste)	0.0065 (total input coal)
Tar	0.20 (total waste)	0.025 (total input coal)
Gas liquor	Total waste - ash - carbon - sulfur	1.5 (total input coal)

REFERENCES

1. U.S. Environmental Protection Agency, Evaluation of Background Data Relating to New Source Performance Standards for Lurgi Gasification, EPA-600/7-77-057, June 1977.

2. R.G. Oldham and R. G. Wetherold, Assessment, Selection and Development of Procedures for Determining the Environmental Acceptability of Synthetic Fuel Plants based on Coal, Appendix 1, Radian Corp., FE-1795-3 (Pt. 1), revised May 1977.

3. D. W. Koppenaal, Trace Element Studies on Coal Gasification Process Streams, Ph.D. dissertation, University of Missouri-Columbia, TID-29022, Sept. 1978.

4. U.S. Environmental Protection Agency, Environmental Assessment Data Base for High-Btu Gasification Technology, Vol. 1-3, EPA-600/7-78-186a, Sept. 1978.

5. C. F. Blazek, N. R. Baker, and R. R. Tison, High-Btu Coal Gasification Processes, ANL/CES/TE 79-2, Jan. 1979.

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7. M. H. Somerville, J. L. Elder, and R. G. Todd, Trace Elements: Analysis of Their Potential Impact from a Coal Gasification Facility, from Technology and Use of Lignite, symposium sponsored by U.S. ERDA, GFERC/1C-77/1, May 1977.

8. J. Antizzo, Background Material for the Workshop on Health and Environmental Effects of Coal Gasification and Liquefaction Technologies, M78-58, MITRE Corporation, McLean, VA, 1978.

APPENDIX 4A

DETERMINATION OF SOLID WASTE CHARACTERISTICS: TOTAL SOLID WASTE, WATER, CARBON, SULFUR, ASH

Descriptions of the estimation of the solid waste streams of interest and their non-trace components (water, carbon, sulfur, and ash) are given below. In most cases, it was determined that the quantity involved is best described as a fraction of the input quantity of the element or of the total coal. In this appendix, the "ash" in the coal will be differentiated from the "ash" remaining in the gasifier after gasification by referring to the latter as "bottom ash."

4A.1 Total Solid Waste

Bottom Ash (wet). The bottom ash in this module is calculated as the sum of its major components, i.e.,

BOTTOM ASH = ASH + CARBON + SULFUR + WATER.

Oil. Table 4A.1 shows the input coal characteristics and waste production information for several types of coal. The oil produced is seen to range from 0.45 to 1.96 tons per 100 tons of the input coal type (i.e., the amount of oil produced is equal to 0.45 to 1.96% of the amount of input coal). Since most of these range from 0.45 to 0.76, the total oil produced was taken to be 0.65% of the input coal, i.e.,

Total Oil = $0.0065 \cdot Q$

where Q = total input coal.

Table 4A.1
Coal Characteristics, Total Waste Streams, Water Content*

	Coal Reference No.**						
	1	2	3	4	5	6	9
Carbon content of input coal	50.56	64.15	64.11	74.15	48.21	45.74	39.05
Ash content of input coal	9.71	9.07	8.10	7.73	29.07	4.75	4.20
Sulfur content of input coal	1.092	2.810	3.135	2.519	0.396	0.807	0.799
Bottom ash production rate***	12.0	10.0	9.2	8.1	31.0	10.0	-
Bottom ash produced (dry)	9.036	8.977	8.102	7.729	28.52	6.402	-
Oil production rate	2.6	0.5	0.6	0.8	0.8	0.8	0.8
Oil produced	1.958	0.449	0.528	0.763	0.736	0.512	0.492
% Water	22.3	4.3	5.4	15.4	-	-	-
Tar production rate	2.6	2.7	3.5	3.8	1.5	1.5	1.5
Tar produced	1.958	2.424	3.082	3.626	1.380	0.960	0.922
% Water	30.0	26.7	10.4	11.9	-	-	-
Gas liquor production rate	93.0	211.0	177.0	260.0	106.0	153.0	153.0
Gas liquor produced	70.03	189.41	155.87	248.09	97.52	97.95	94.00

*All quantities in tons/100 tons raw input coal unless otherwise noted.
**Data calculated from References 4 and 6.
***Production rates given as percentage of amount of input coal (dry basis).

Tar. Table 4A.1 shows that tar production is from 0.92 to 3.6% of theinput coal. A "good" estimate of tar production is taken as 2.5% of the inpucoal,

TOTAL TAR = 0.025 • Q.

Gas Liquor. Gas liquor production ranges from about 0.7 to 2.5 times the amount of total input coal. A rough average was taken to be 1.5 times the input coal quantity,

TOTAL GAS LIQUOR = 1.5 • Q.

4A.2 Water

Bottom Ash. Water retained in the bottom ash waste stream is equal toapproximately one-fifth of the dry weight of the bottom ash[2]:

WATER = 0.20 • (ASH + CARBON + SULFUR).

Oil. The amount of water in the oil ranges from 4.3 to 22.3%. An average of 12% is taken as "typical":

WATER = 0.12 · Oil.

Tar. Water content of tar ranges from 10 to 30%. The median of 20% was taken as a "good" estimate:

WATER = 0.20 · Tar.

Gas Liquor. Since gas liquor is basically water, water content is assumed to be the total gas liquor produced minus its major dry components,

WATER = GAS LIQUOR - ASH - CARBON - SULFUR.

4A.3 Carbon

Table 4A.2 gives the distribution of carbon over three of the waste streams. Usable data are not available on the carbon content of gas liquor.

Table 4A.2
Carbon Distribution*

Component	Coal Reference No.** 1	2	3	4
Carbon content of input raw coal	50.56	64.15	64.11	74.15
Carbon - % of bottom ash	6.5	4.3	2.9	7.6
Carbon in bottom ash	0.587	0.386	0.235	0.587
% of input carbon in bottom ash	1.16	0.60	0.37	0.79
Carbon - % of oil (water-free basis)	81.3	84.8	84.9	87.3
Carbon in oil	1.237	0.365	0.424	0.564
% of input carbon in oil	2.45	0.57	0.66	0.76
Carbon - % of tar (dry basis)	83.06	85.48	85.85	88.51
Carbon in tar	1.138	1.519	2.371	2.827
% of input carbon in tar	2.25	2.37	3.70	3.81

*All quantities given in tons/100 tons raw input coal unless otherwise noted.
**Data calculated from Reference 4.

Bottom Ash. Bottom ash carbon content ranges from 0.37 to 1.16 percent of the input carbon. Carbon captured in bottom ash is assumed to be approximately 0.8% of the input carbon,

CARBON = 0.008 · INPUT CARBON.

Oil. An estimate of 1% of the input carbon gets captured in the oil was assumed after inspection of Table 4A.2,

CARBON = 0.01 · INPUT CARBON.

Tar. An average of 3% of the input carbon seems to get captured in the tar,

CARBON = 0.03 · INPUT CARBON.

Gas Liquor. No usable data are available on carbon in gas liquor; a token estimate of 0.01% is assumed since almost all carbon is probably removed in tar and oil separation.

4A.4 Sulfur

Table 4A.3 gives the sulfur distribution across three of the solid waste streams. No usable data are available on the sulfur content of gas liquor. 2.26% of the sulfur is captured in the solid waste streams. About 96% is recovered in the sulfur process (Reference 1). The rest is assumed to escape with product and emission gases. Pyritic (inorganic) sulfur is assumed to follow the same distribution as total sulfur.

Bottom Ash. About 0.25% of the input sulfur is indicated as captured in the bottom ash, i.e.,

SULFUR = 0.0025 · INPUT SULFUR.

Table 4A.3
Sulfur Distribution*

Component	Coal Reference No.** 1	2	3	4
Sulfur content of input raw coal	1.092	2.810	3.135	2.519
Sulfur - % of bottom ash	0.061	0.054	0.029	0.029
Sulfur in bottom ash	0.0055	0.0048	0.0023	0.0022
% of input sulfur in bottom ash	0.50	0.17	0.07	0.09
Sulfur - % of oil (water free basis)	0.5	2.4	2.3	1.5
Sulfur in oil	0.0076	0.0103	0.0115	0.0097
% of input sulfur in oil	0.70	0.37	0.37	0.39
Sulfur - % of tar (dry basis)	0.28	1.7	2.4	1.5
Sulfur in tar	0.0038	0.0302	0.0663	0.0579
% of input sulfur in tar	0.35	1.07	2.11	1.90

*All quantities given in tons/100 tons raw input coal unless otherwise noted
**Data calculated from Reference 4.

Oil. Inspection of Table 4A.3 seems to indicate that 0.5% of the input sulfur is captured in the oil.

SULFUR = 0.005 · INPUT SULFUR.

Tar. The range of sulfur contained in the tar seems to show that 1.5% of the input amount of sulfur may be captured in the tar.

SULFUR = 0.015 · INPUT SULFUR.

Gas Liquor. As with the amount of carbon in the gas liquor, sulfur is given a token fraction that is assumed captured in the gas liquor.

SULFUR = 0.0001 · INPUT SULFUR.

4A.5. Ash

Table 4A.4 gives the distribution of the ash content of coal through the bottom ash, tar, and oil streams. No data are available on the ash content of gas liquor; as with carbon and sulfur, the gas liquor is assigned a token negligible amount of captured ash. Since the total amount of ash found in the

Table 4A.4
Ash Distribution*

Component	Coal Reference No.** 1	2	3	4
Ash content of input raw coal	9.71	9.07	8.10	7.73
Ash in bottom ash***	8.4435	8.5862	7.8647	7.1398
% of input ash in bottom ash	86.96	94.67	97.10	92.36
Ash - % of oil (water- free basis)	0.03	0.01	0.01	0.01
Ash in oil	0.00046	0.00004	0.00005	0.00006
% of input ash in oil	0.0047	0.0004	0.0006	0.0008
Ash - % of tar (dry basis)	0.05	0.03	0.01	0.01
Ash in tar	0.0007	0.0005	0.0003	0.0003
% of input ash in tar	0.0072	0.0055	0.0037	0.0039

*All quantities given in tons/100 tons raw input coal unless otherwise noted.
**Data calculated from Reference 4.
***By subtraction of carbon and sulfur from total bottom ash.

data is always several percent below 100% of the coal ash content, the numbers had to be increased slightly from what the data indicate is the "true" amount of captured ash in the waste streams. The following are the estimates for ash retention:

BOTTOM ASH: ASH = 0.9924 · INPUT ASH
OIL: ASH = 0.0025 · INPUT ASH
TAR ASH = 0.005 · INPUT ASH
GAS LIQUOR: ASH = 0.0001 · INPUT ASH

4A.6. Sulfur Recovery

Although marketable sulfur is usually produced through the sulfur recovery process, and therefore the sulfur cannot really be considered a waste stream, it is included in this module as such. It is assumed that the stream is pure sulfur; therefore the total solid waste vector element will be equal to the total sulfur element. As mentioned before, 96% of the input coal sulfur content is assumed to be recovered in this process. All other elements in the stream are 0.

APPENDIX 4B

DETERMINATION OF SOLID WASTE CHARACTERISTICS: FRACTIONATION FACTORS OF TRACE ELEMENTS

As mentioned previously, data on trace elements are highly variable. Some attempts have been made to follow the paths of the trace elements as they go through the gasification process; however, because of analytic measurement error, poor sampling procedures (from a strict testing standpoint), or unknown factors, recovered mass balances of trace elements of from 10 to over 2000 percent are not unknown (or uncommon).

An attempt is made here to split the trace elements so that their total mass balance is accounted for in the solid waste streams. Although some of the trace elements are probably lost to catalysts (in shift reaction and methanation) and some to fugitive air emissions, these amounts are assumed to be negligible and, as far as this module is concerned, nonexistent. This assumption is not without precedent, as it has been made in other analyses (Reference 1, p. 36; Reference 7, Table 5; Reference 4, Appendix 4A).

While varying amounts of the total mass of the trace elements in the input coal have been found, mercury and selenium are consistently short of a total mass balance. Therefore, these two are assumed to have lost some amount to unknown processes and are not completely accounted for in the solid waste streams. All other elements have been normalized so that 100% of the input mass has come out in the solid waste streams.

Table 4B.1 gives the input coal content of trace elements for which trace element distributions have been calculated. Tables 4B.2 to 4B.5 give the amounts of the elements (as fraction of input element) in the solid waste

Table 4B.1
Coal Content of Trace Elements (ppm)

	Coal Reference No.					
Element	1	2	3	5	6	None
Sb	-	0.1	0.2	<0.5	0.11	0.18
As	1.0	1.0	2.0	3.5	24.85	5.26
Be	0.75	1.6	2.0	2.5	1.06	0.18
Cd	0.56	<0.4	-	<0.1	0.63	0.66
Cr	10.0	20.0	15.0	-	3.7	3.48
Cu	9.5	12.0	10.0	-	3.8	6.96
Fe	4520.0	13470.0	23160.0	10120.0	3840.0	5214.0
Pb	12.0	10.0	28.0	15.0	20.0	1.77
Mg	1730.0	360.0	350.0	2760.0	1660.0	2547.0
Mn	3.1	20.0	22.0	500.0	31.0	46.45
Hg	0.14	1.1	0.2	<0.1	0.07	0.13
Ni	8.0	14.0	32.0	40.0	3.55	4.4
Se	0.33	1.3	1.3	0.3	1.15	0.26
Ag	0.06	-	-	-	<0.1	0.07
Tl	-	-	-	-	-	0.07
Th	-	-	-	-	-	2.63
U	0.88	-	-	-	0.635	2.63
Zn	5.0	43.0	200.0	-	12.0	4.40
Reference	6	6	6	6	6	4

- Indicates data not available.

Table 4B.2
Fraction of Input Trace Elements in Bottom Ash

	Coal Reference No.*									
Element	1	2	2	3	5	6	6	None	None**	None**
Sb	-	0.18	3.77	7.70	0.29	0.58	19.21	0.10	0.40(0.50)	1.63 (1.00)
As	1.96	0.01	0.27	0.01	0.08-0.16	0.15	0.19	0.01	0.36(0.27)	1.02 (0.91)
Be	0.34	0.79	0.67	0.81	0.006	0.30	0.36	0.80	0.01(0.33)	2.46 (0.99)
Cd	0.39	0.07	0.36	-	0.29	0.10	0.05	-	0.40(0.52)	0.06 (0.15)
Cr	3.98	3.37	0.95	3.20	-	0.69	2.42	3.00	-	2.93 (0.98)
Cu	1.24	1.79	0.43	2.21	-	0.84	0.45	2.00	-	0.28 (0.94)
Fe	1.57	0.80	0.96	0.48	0.99	-	1.28	-	-	1.10 (0.99)
Pb	0.30	0.86	0.40	0.58	0.95	0.64	0.19	0.80	1.80(0.94)	2.35 (0.88)
Mg	1.22	1.50	0.90	0.97	1.05	-	1.62	-	-	1.29 (0.99)
Mn	23.03	0.90	8.34	1.12	1.14	-	1.57	0.90	1.54(0.99)	1.10 (0.99)
Hg	0.02	0.003	0.004	0.01	-	0.09	0.05	0.01	0.40(0.52)	0.03 (0.01)
Ni	2.26	2.92	0.57	1.14	1.07-1.43	0.45	0.45	1.25	1.54(0.994)	0.42 (0.93)
Se	0.60	-	0.07	-	-	0.08	0.03	-	-	0.14 (0.14)
Ag	0.35	-	-	-	-	0.45	0.64	-	-	1.10 (1.00)
Tl	-	-	-	-	-	-	-	-	-	5.50 (1.00)
Th	-	-	-	-	-	-	-	-	-	1.24 (0.99)
U	1.33	-	-	-	-	0.60	0.71	-	-	0.19 (0.94)
Zn	0.58	0.98	0.84	0.65	-	0.00 2	0.05	0.90	-(1.00)	0.17 (0.75)
Reference	6	6	6	6	6	6	6	4	4	3

- Indicates data not available.

* Coals No. 2 and No. 6 each had two separate analyses performed on them.

** Numbers in parenthesis are fractions which have been normalized to 100% across the four waste streams.

Table 4B.3
Fraction of Input Trace Elements in Oil

	Coal Reference No.				
Element	**5**	**6**	**9**	**None***	**None***
Sb	0.49	-	0.002	0.005 (0.006)	0 (0)
As	0.221-0.553	0.024-0.036	0.005	0.052 (0.039)	0.036 (0.032)
Be	0.0002-0.0003	0.0005-0.008	0.001	0.0001 (0.003)	0 (0)
Cd	0.191	0.035	0.020	0.011 (0.014)	0.006 (0.016)
Cr	-	0.024-0.105	0.0003	-	0.009 (0.003)
Cu	-	0.014-0.076	0.004	-	0.002 (0.007)
Fe	-	0.0007	-	-	0.0002 (0.0002)
Pb	0.004-0.008	0.012-0.347	0.0002	0.0002 (0.001)	0.0003 (0.007)
Mg	-	0.0001	-	-	0.0001 (0.0001)
Mn	NG	0.0005-0.002	-	NG	0.0001 (0.0001)
Hg	0.099	0.123-0.221	0.033	0.005 (0.006)	0.011 (0.005)
Ni	0.002-0.003	0.015-0.076	0.005	0.0001 (NG)	0.003 (0.007)
Se	-	0.008-0.009	0.0003	-	0.005 (0.013)
Ag	-	-	1.720	-	0 (0)
Tl	-	-	-	-	0 (0)
Th	-	-	-	-	0 (0)
U	-	-	0.03	-	0 (0)
Zn	-	0.006-0.122	0.001	-	0.004 (0.016)
Reference	6	6	6	4	3

NG indicates negligible amount (<.0001).

- Indicates data not available.

* Numbers in parenthesis are fractions which have been normalized to 100% across the four waste streams.

Table 4B.4
Fraction of Input Trace Elements in Tar

	Coal Reference No.						
Element	5	6	9	None*		None*	
Sb	0.128	-	0.009	0.03	(0.38)	0	(0)
As	0.056-0.139	0.014	0.009	0.025	(0.019)	0.048	(0.043)
Be	0.071	-	0.005	0.005	(0.17)	0.022	(0.009)
Cd	0.052	0.034	0.033	0.005	(0.006)	0.017	(0.045)
Cr	-	0.05 -0.214	0.0009	-		0.054	(0.018)
Cu	-	0.035-0.186	0.0003	-		0.016	(0.053)
Fe	-	0.016	-	-		0.011	(0.010)
Pb	0.454	0.007-0.203	0.003	0.082	(0.043)	0.291	(0.109)
Mg	-	0.004	-	-		0.011	(0.009)
Mn	0.0004	0.013-0.056	-	NG		0.008	(0.007)
Hg	0.649	3.64-6.55	0.054	0.049	(NG)	0.821	(0.382)
Ni	0.007	0.038-0.186	0.06	0.0005	(0.0003)	0.026	(0.057)
Se	-	0.006-0.008	0.009	-		0.011	(0.028)
Ag	-	-	0.562	-		0	(0)
Tl	-	-	-	-		0	(0)
Th	-	-	-	-		0.008	(0.034)
U	-	0.142-0.526	0.253	-		0.013	(0.062)
Zn	-	0.004-0.089	0.031	-		0.014	(0.011)
Reference	6	6	6	4		3	

NG indicates negligible amount (<.0001).
- indicates data not available.
* Numbers in parenthesis are fractions which have been normalized to 100% across the four waste streams.

Table 4B.5
Fraction of Input Trace Elements in Gas Liquor

	Coal Reference No.				
Element	1	6	9	None*	None*
Sb	-	-	0.09	0.36 (0.45)	0 (0)
As	0.008-1.75	0.003-0.005	0.282	0.90 (0.672)	0.019 (0.017)
Be	0.193-0.220	-	0.026	0.016 (0.53)	0 (0)
Cd	0.088-0.226	0.311	0.133	0.35 (0.455)	0.302 (0.794)
Cr	0.057-0.228	0.003-0.014	0.0004	-	0.006 (0.002)
Cu	0.070-0.078	0.003-0.017	0.012	-	0.002 (0.005)
Fe	-	NG	-	-	0.0001 (0.0001)
Pb	0.007-0.165	0.0003-0.007	0.003	0.032 (0.017)	0.003 (0.001)
Mg	-	0.0002	-	-	0.0002 (0.0002)
Mn	0.002-0.003	1.86-3.34	-	0.32 (0.002)	0.001 (0.001)
Hg	0.229-0.355	1.86-3.34	0.015	0.32 (0.416)	1.288 (0.599)
Ni	0.025-.0.175	0.001-0.005	0.016	0.006 (0.004)	0.001 (0.003)
Se	0.106	0.003-0.004	2.21	-	0.006 (0.015)
Ag	0.20	-	6.27	-	0 (0)
Tl	-	-	-	-	0 (0)
Th	-	-	-	-	0 (0)
U	0.119	-	0.063	-	0 (0)
Zn	0.005-0.021	0.016-0.327	0.342	-	0.045 (0.103)
Reference	6	6	6	4	3

NG indicates negligible amount (<.0001).
- Indicates data not available.
* Numbers in parenthesis are fractions which have been normalized to 100% across the four waste streams.

streams which were found for some or all of these coals, as data were available. Tables 4B.2 to 4B.5 also have some data for the references where this fraction was already calculated. Note that when the numbers are greater than one, more of that element has been found in the waste stream then was in the input coal. Some authors explain this by saying that the extra elements found are from the construction materials in the gasifier system[3]. The magnitude of the amounts involved preclude this as an explanation.

After examining the data in Tables 4B.2 to 4B.5, an attempt was made to distribute the trace elements across the waste streams such that there was some agreement with the data and that the mass of the elements was totally accounted for (except for those elements noted above). Different observations of the data at different times have yielded varying results for some of the trace elements, although the difference was in the size of the coefficients: in general, the relative distribution of each element across the waste stream was not changed significantly. Certainly, almost any reasonable estimate of a coefficient can be no better or worse than those decided upon here. Table 4.2 in the main report gives the latest estimation of the coefficients.

Special Notes: No data were available on the distributions of radium-226, radium-228 or lead-210. Also, very few data were available for uranium and thorium. It was therefore decided that all radioactive elements follow the same distribution, except for lead-210 which is distributed as Pb.

There is only one measurement for thallium, which indicates that all of it gets captured in the bottom ash. There is no reason to assume that all of the thallium is captured here, although the bulk of it may be; the coefficients for thallium reflect this.

APPENDIX 4C

DESCRIPTION OF COMPUTER MODULE

The coal gasification solid waste module consists of one subroutine and a data file containing the fraction of the waste components that are removed to the solid waste. The module is set into motion by a call to LURGI:

CALL LURGI (Q, COAL, CHAR, OIL, TAR, LIQUOR, SREC),

where

Q = total mass of input coal
COAL = input coal characteristic vector
CHAR = bottom ash output characteristic vector
OIL = oil output characteristic vector
TAR = tar output characteristic vector
LIQUOR = gas liquor output characteristic vector
SREC = sulfur recovery output characteristic vector

The subroutine calculates the solid waste characteristics of each waste stream and prints them out (see Appendix 4D for sample output). The data file contains the coefficients of all elements that are removed at a constant rate and can be calculated by a simple multiplication. All elements in the input vector that are empty, are not applicable to this module, or are calculated other than by a single multiplication (i.e., water and some total wastes) have corresponding coefficients of zero.

All calculations (including empty and nonapplicable elements) are done through DO loops in the module. The water and total solid waste elements are calculated separately.

The module prints out the input coal and output waste vectors (applicable elements only). If this printout is not desired at some future time, the printout section can simply be removed with no effect on the solid waste calculations. All vectors are returned to the calling program intact, inlcuding the input coal characteristics.

The data file is presently read in as "TAPE1".

APPENDIX 4D

COMPUTER CODE AND SAMPLE OUTPUT

This section sets out the computer code used for the coal gasification module and the data file of coefficients, with a sample input and the resulting output. Table 4D.1 gives the coal characteristics used as input. The quantity of coal (Q) in the input is 100,000 tons.

At present the main program of the code is used only to set the input variables.

Table 4D.1
Input Characteristics of Coal

Element	Input Quantity (tons)
Ash	18700.00
Sulfur	3000.00
Antimony	0.07
Arsenic	2.70
Beryllium	0.50
Cadmium	0.125
Chromium	3.00
Copper	1.18
Iron	2700.00
Lead	1.14
Magnesium	118.00
Manganese	7.40
Mercury	0.017
Nickel	2.00
Selenium	0.02
Silver	0.01
Thallium	0.66
Zinc	1.69
Uranium	0.07
Thorium	0.66
Pyritic sulfur	1870.00
Carbon	64100.00
Btu	2.3×10^{12}

```
      PROGRAM CLL(TAPE1,OUTPUT,TAPE2=OUTPUT)
      DIMENSION COAL(50)
      REAL CHAR(50),OIL(50),TAR(50),LIQUOR(50),SREC(50)
      Q=100000
      COAL(1)=18700.
      COAL(2)=3000.
      COAL(3)=.07
      COAL(4)=2.7
      COAL(5)=.5
      COAL(6)=.125
      COAL(7)=3.
      COAL(8)=1.18
      COAL(9)=2700
      COAL(10)=1.14
      COAL(11)=118.
      COAL(12)=7.4
      COAL(13)=.017
      COAL(14)=2.
      COAL(15)=.02
      COAL(16)=.01
      COAL(17)=.66
      COAL(18)=1.69
      COAL(19)=.07
      COAL(20)=.66
      DO 10 I=21,38
      COAL(I)=0.
   10 CONTINUE
      COAL(39)=1870.
      COAL(40)=64100
      COAL(41)=2.3E12
      DO 20 I=42,50
      COAL(I)=0.
   20 CONTINUE
      CALL LURGI(Q,COAL,CHAR,OiL,TAR,LIQUOR,SREC)
      STOP
      END
```

```
      SUBROUTINE LURGI(Q,COAL,CHAR,OIL,TAR,LIQUOR,SREC)
      DIMENSION COAL(50),CHAR(50),OIL(50),TAR(50),LIQUOR(50),SREC(50)
      REAL LIQUOR,CHARC(50),OILC(50),TARC(50),LIQUORC(50),SRECC(50)
C    * COEFFICIENTS FOR DETERMINING ELEMENTAL SPLIT BETWEEN
C    * THE OUTPUT PRODUCT AND WASTE STREAMS READ IN
      READ(1,1000)(CHARC(I),OILC(I),TARC(I),LIQUORC(I),SRECC(I),I=1,50)
1000  FORMAT(F9.5,4F10.5)
C    * CALCULATION OF INPUT RA-226,RA-228 & PB-210 IF NOT GIVEN
      IF(COAL(21) .EQ. 0.)COAL(21)=3.38E-7*COAL(19)
      IF(COAL(22) .EQ. 0.)COAL(22)=4.01E-10*COAL(20)
      IF(COAL(23) .EQ. 0.)COAL(23)=4.37E-9*COAL(19)
C    * CALCULATION OF AMOUNT OF EACH ELEMENT IN EACH OUTPUT STREAM
      DO 10 I=1,24
      CHAR(I)=CHARC(I)*COAL(I)
      OIL(I)=OILC(I)*COAL(I)
      TAR(I)=TARC(I)*COAL(I)
      LIQUOR(I)=LIQUORC(I)*COAL(I)
      SREC(I)=SRECC(I)*COAL(I)
   10 CONTINUE
C    * ELEMENTS NOT APPLICABLE TO GASIFICATION SET TO ZERO
      DO 20 I=26,33
      CHAR(I)=0.
      OIL(I)=0.
      TAR(I)=0.
      LIQUOR(I)=0.
      SREC(I)=0.
   20 CONTINUE
      DO 30 I=35,50
      CHAR(I)=CHARC(I)*COAL(I)
      OIL(I)=OILC(I)*COAL(I)
      TAR(I)=TARC(I)*COAL(I)
      LIQUOR(I)=LIQUORC(I)*COAL(I)
      SREC(I)=SRECC(I)*COAL(I)
   30 CONTINUE
C    * CALCULATION OF WATER CONTENT AND TOTAL QUANTITY OF BOTTOM ASH
      CHAR(34)=.2*(CHAR(1)+CHAR(2)+CHAR(40))
      CHAR(25)=CHAR(1)+CHAR(2)+CHAR(40)+CHAR(34)
C    * CALCULATION OF TOTAL QUANTITY AND WATER CONTENT OF OIL
      OIL(25)=.01*Q
      OIL(34)=.12*OIL(25)
C    * CALCULATION OF TOTAL QUANTITY AND WATER CONTENT OF TAR
      TAR(25)=.03*Q
      TAR(34)=.20*TAR(25)
C    * CALCULATION OF TOTAL QUANTITY AND WATER CONTENT OF GAS LIQUOR
      LIQUOR(25)=1.5*Q
      LIQUOR(34)=LIQUOR(25)-LIQUOR(1)-LIQUOR(2)-LIQUOR(40)
C    * CALCULATION OF TOTAL QUANTITY AND WATER CONTENT OF SULFUR PRODUCT
      SREC(25)=SREC(2)
      SREC(34)=0.
C
C
C          PRINT OUT OF DATA
C
C
      WRITE(2,2000)Q,COAL(1),CHAR(1),OIL(1),TAR(1),LIQUOR(1),SREC(1),
     -COAL(2),CHAR(2),OIL(2),TAR(2),LIQUOR(2),SREC(2),
```

```
     -COAL(3),CHAR(3),OIL(3),TAR(3),LIQUOR(3),SREC(3),
     -COAL(4),CHAR(4),OIL(4),TAR(4),LIQUOR(4),SREC(4)
 2000 FORMAT(1H1,5X,*INPUT COAL:*2X,E12.5/1X,*ELEMENT*,T16,*INPUT COAL*,
     -T31,*ASH*,T46,*OIL*,T61,*TAR*,T76,*LIQUOR*,T91,*SULFUR RECOVERY*/
     -1X,105(*-*)/
     -1X,*ASH*,T16,E12.5,5(3X,E12.5)/
     -1X,1H*,*SULFUR*,T16,E12.5,5(3X,E12.5)/
     -1X,*ANTIMONY*,T16,E12.5,5(3X,E12.5)/
     -1X,*ARSENIC*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2001)COAL(5),CHAR(5),OIL(5),TAR(5),LIQUOR(5),SREC(5),
     -COAL(6),CHAR(6),OIL(6),TAR(6),LIQUOR(6),SREC(6),
     -COAL(7),CHAR(7),OIL(7),TAR(7),LIQUOR(7),SREC(7),
     -COAL(8),CHAR(8),OIL(8),TAR(8),LIQUOR(8),SREC(8)
 2001 FORMAT(1X,*BERYLLIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*CADMIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*CHROMIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*COPPER*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2002)COAL(9),CHAR(9),OIL(9),TAR(9),LIQUOR(9),SREC(9),
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     -COAL(11),CHAR(11),OIL(11),TAR(11),LIQUOR(11),SREC(11),
     -COAL(12),CHAR(12),OIL(12),TAR(12),LIQUOR(12),SREC(12)
 2002 FORMAT(1X,*IRON*,T16,E12.5,5(3X,E12.5)/
     -1X,*LEAD*,T16,E12.5,5(3X,E12.5)/
     -1X,*MAGNESIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*MANGANESE*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2003)COAL(13),CHAR(13),OIL(13),TAR(13),LIQUOR(13),SREC(13)
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     -COAL(15),CHAR(15),OIL(15),TAR(15),LIQUOR(15),SREC(15),
     -COAL(16),CHAR(16),OIL(16),TAR(16),LIQUOR(16),SREC(16)
 2003 FORMAT(1X,1H*,*MERCURY*,T16,E12.5,5(3X,E12.5)/
     -1X,*NICKEL*,T16,E12.5,5(3X,E12.5)/
     -1X,1H*,*SELENIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*SILVER*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2004)COAL(17),CHAR(17),OIL(17),TAR(17),LIQUOR(17),SREC(17)
     -,COAL(18),CHAR(18),OIL(18),TAR(18),LIQUOR(18),SREC(18),
     -COAL(19),CHAR(19),OIL(19),TAR(19),LIQUOR(19),SREC(19),
     -COAL(20),CHAR(20),OIL(20),TAR(20),LIQUOR(20),SREC(20)
 2004 FORMAT(1X,*THALLIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*ZINC*,T16,E12.5,5(3X,E12.5)/
     -1X,*URANIUM*,T16,E12.5,5(3X,E12.5)/
     -1X,*THORIUM-232*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2005)COAL(21),CHAR(21),OIL(21),TAR(21),LIQUOR(21),SREC(21)
     -,COAL(22),CHAR(22),OIL(22),TAR(22),LIQUOR(22),SREC(22),
     -COAL(23),CHAR(23),OIL(23),TAR(23),LIQUOR(23),SREC(23),
     -COAL(25),CHAR(25),OIL(25),TAR(25),LIQUOR(25),SREC(25)
 2005 FORMAT(1X,*RADIUM-226*,T16,E12.5,5(3X,E12.5)/
     -1X,*RADIUM-228*,T16,E12.5,5(3X,E12.5)/
     -1X,*LEAD-210*,T16,E12.5,5(3X,E12.5)/
     -1X,*TOTAL WASTE*,T16,E12.5,5(3X,E12.5))
      WRITE(2,2006)COAL(34),CHAR(34),OIL(34),TAR(34),LIQUOR(34),SREC(34)
     -,COAL(39),CHAR(39),OIL(39),TAR(39),LIQUOR(39),SREC(39),
     -COAL(40),CHAR(40),OIL(40),TAR(40),LIQUOR(40),SREC(40)
 2006 FORMAT(1X,*WATER*,T16,E12.5,5(3X,E12.5)/
     -1X,1H*,*PYRITIC SULFUR*,T16,E12.5,5(3X,E12.5)/
     -1X,*CARBON*,T16,E12.5,5(3X,E12.5)//
     -1X,1H*,*-DOES NOT EQUAL 100 PERCENT BECAUSE OF LOSS TO PRODUCT AND
     -/OR EFFLUENT GAS.*//)
      RETURN
      END
```

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.9924    .0025    .005     .0001    0.
.0025    .005     .015     .0001    .96
.5       .01      .04      .45      0.
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.59      .03      .03      .35      0.
.93      .01      .05      .01      0.
.96      .01      .02      .01      0.
.98      .0005    .019     .0005    0.
.87      .01      .11      .01      0.
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.98      .005     .01      .005     0.
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.80      .03      .10      .07      0.
.80      .03      .10      .07      0.
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0.       0.       0.       0.       0.
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0.       0.       0.       0.       0.
0.       0.       0.       0.       0.
.0025    .005     .015     .0001    .96
.008     .01      .03      .0001    0.
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0.       0.       0.       0.       0.
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0.       0.       0.       0.       0.
0.       0.       0.       0.       0.
```

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   INPUT COAL:      .10000E+06
ELEMENT          INPUT COAL     ASH           OIL           TAR           LIQUOR         SULFUR RECOVERY
----------------------------------------------------------------------------------------------------------
ASH               .18700E+05   .18558E+05   .46750E+02   .93500E+02   .18700E+01    0.
*SULFUR           .30000E+04   .75000E+01   .15000E+02   .45000E+02   .30000E+00     .28800E+04
ANTIMONY          .70000E-01   .35000E-01   .70000E-03   .28000E-02   .31500E-01    0.
ARSENIC           .27000E+01   .12150E+01   .13500E+00   .13500E+00   .12150E+01    0.
BERYLLIUM         .50000E+00   .46500E+00   .50000E-02   .15000E-01   .15000E-01    0.
CADMIUM           .12500E+00   .73750E-01   .37500E-02   .37500E-02   .43750E-01    0.
CHROMIUM          .30000E+01   .27900E+01   .30000E-01   .15000E+00   .30000E-01    0.
COPPER            .11800E+01   .11328E+01   .11800E-01   .23600E-01   .11800E-01    0.
IRON              .27000E+04   .26460E+04   .13500E+01   .51300E+02   .13500E+01    0.
LEAD              .11400E+01   .99180E+00   .11400E-01   .12540E+00   .11400E-01    0.
MAGNESIUM         .11800E+03   .11564E+03   .59000E-01   .22420E+01   .59000E-01    0.
MANGANESE         .74000E+01   .72520E+01   .74000E-02   .11840E+00   .22200E-01    0.
*MERCURY          .17000E-01   .51000E-03   .85000E-03   .93500E-02   .59500E-02    0.
NICKEL            .20000E+01   .19000E+01   .20000E-01   .60000E-01   .20000E-01    0.
*SELENIUM         .20000E-01   .20000E-02   .20000E-03   .20000E-03   .20000E-03    0.
SILVER            .10000E-01   .97000E-02   .10000E-03   .10000E-03   .10000E-03    0.
THALLIUM          .66000E+00   .64680E+00   .33000E-02   .66000E-02   .33000E-02    0.
ZINC              .16900E+01   .15379E+01   .33800E-01   .67600E-01   .50700E-01    0.
URANIUM           .70000E-01   .56000E-01   .21000E-02   .70000E-02   .49000E-02    0.
THORIUM-232       .66000E+00   .52800E+00   .19800E-01   .66000E-01   .46200E-01    0.
RADIUM-226        .23660E-07   .18928E-07   .70980E-09   .23660E-08   .16562E-08    0.
RADIUM-228        .26466E-09   .21173E-09   .79398E-11   .26466E-10   .18526E-10    0.
LEAD-210          .30590E-09   .26613E-09   .30590E-11   .33649E-10   .30590E-11    0.
TOTAL WASTE     0.             .22894E+05   .10000E+04   .30000E+04   .15000E+06     .28800E+04
WATER           0.             .38156E+04   .12000E+03   .60000E+03   .14999E+06    0.
*PYRITIC SULFU    .18700E+04   .46750E+01   .93500E+01   .28050E+02   .18700E+00     .17952E+04
CARBON            .64100E+05   .51280E+03   .64100E+03   .19230E+04   .64100E+01    0.

*-DOES NOT EQUAL 100 PERCENT BECAUSE OF LOSS TO PRODUCT AND/OR EFFLUENT GAS.
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5 SOLID WASTE MODULE FOR THE SRC-II PROCESS COAL LIQUEFACTION

5.1 Introduction

Currently there is a desire to become less dependent on oil as an energy source and to rely more upon abundant domestic coal supplies. Coal has the proven capability of being converted to a gas similar to natural gas, or it can serve as a direct source of energy via combustion. In the latter case, coal can be used in power plants to generate electricity; however, depending upon the type of coal used, there may be a large impact on the environment, especially in terms of sulfur emissions. This in turn could incur high costs to the utility companies for pollution control devices.

The solvent-refined coal (SRC-II) process described herein is a technology which can be used to convert coal to a liquid fuel. Since the main objective of SRC-II is to produce a low-sulfur (<1%) fuel which will minimize sulfur emissions when burned, usually only coals with fairly high sulfur contents are subject to this type of conversion. However, like any other coal technology, the SRC-II process has its own wastes which must be disposed of with as little effect on the environment as possible. To do this as efficiently and economically as possible the wastes must be determined as to both quantity and content.

5.2 The SRC-II Process

Coal conversion to liquid SRC is accomplished through a series of six basic steps and several types of supportive processes[1]. The six basic steps (those used in the actual conversion) are coal pretreatment, hydrogenation, phase (gas) separation, solids/liquid separation, fractionation, and hydrotreating. Supportive processes are generally either by-product recovery, power generation, or waste treatment operations. These include solidification, gas purification, cryogenic separation, sulfur recovery, hydrogen generation, waste water treatment, and auxiliary facilities. See Figure 5.1 for the basic overall flow diagram of a typical SRC-II operation.

SRC-II Process Description

Coal Pretreatment. Coal pretreatment or preparation includes all processes needed to change raw coal into a configuration acceptable to the liquefaction operation. This includes coal receiving, storage, reclaiming and crushing, cleaning, drying, pulverizing, and slurry mixing.

Hydrogenation. The hydrogenation process consists of a slurry preheater and a hydrogen reactor. This is the actual liquefaction of the coal. Subsequent steps in the liquefaction process refine the products made during hydrogenation.

Phase (Gas) Separation. The phase (gas) separation step includes a number of separation techniques (high pressure separation, condensate separation, intermediate flashing, intermediate pressure condensate separation, low pressure condensate separation). In this step, the slurry from hydrogenation is divided into gaseous product and a solids/liquid stream. The output streams from this step are sent to gas purification, fractionation, and solids/liquid separation.

Solids/Liquid Separation. Here the solids/liquid (S/L) stream from phase (gas) separation is divided into two separate streams: solid residue (sent to solidification) and liquid (sent to fractionation).

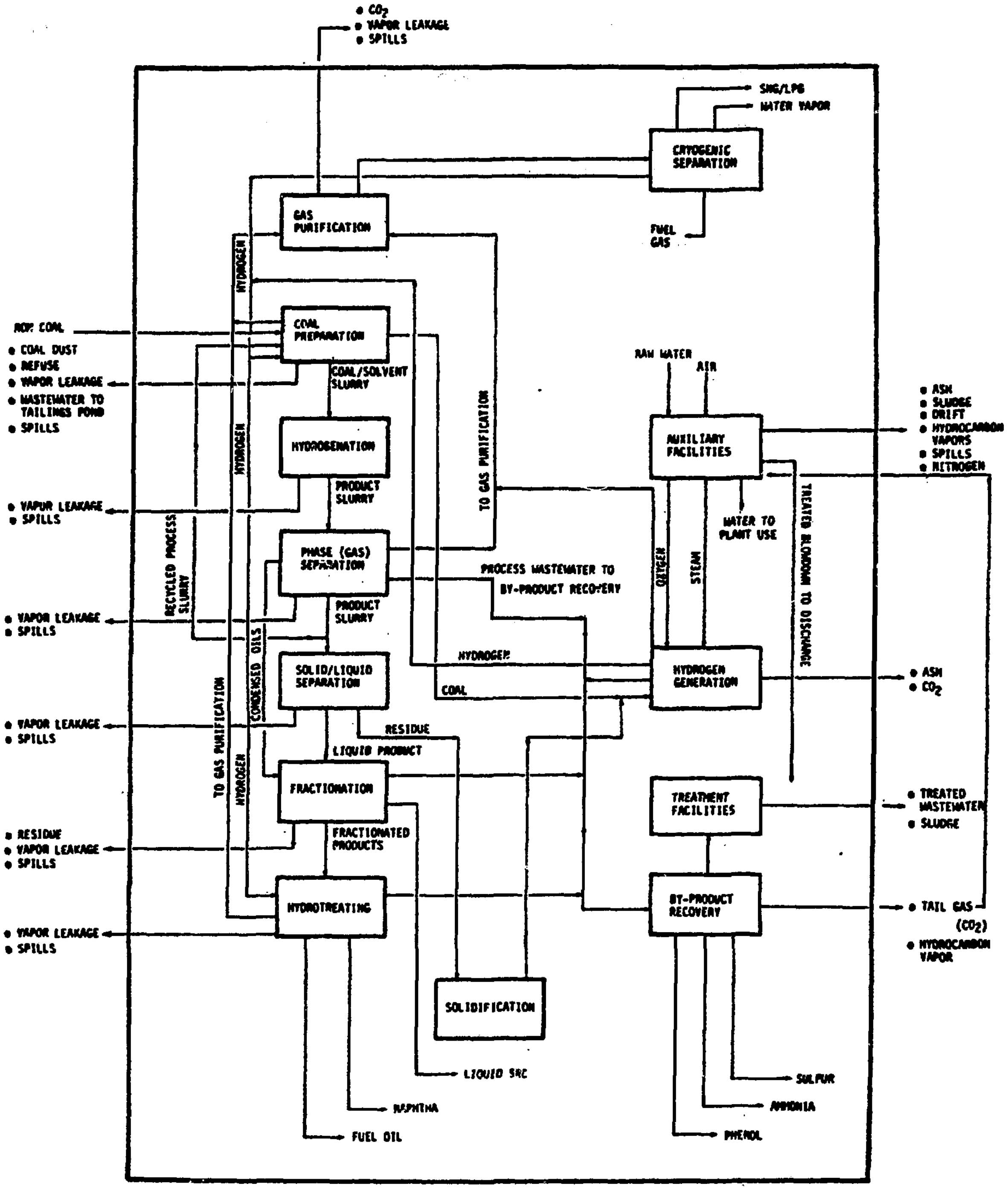

Figure 5.1 Flow diagram of a SRC-II Operation (From Reference 2)

Fractionation. The liquid stream from the previous separation step is subject to a vacuum flash and atmospheric distillation. This performs three functions: (1) separation of the final SRC product from other liquid fractions; (2) combination of light streams (from S/L separation and phase (gas) separation) into light products (sent to hydrotreating); (3) recovery of wash solvent for recycling (to S/L separation).

Solvent Hydrotreating. This process takes the light products from fractionation and refines them to salable commercial products, fuel oil and naphtha. A portion of these products are recycled for use in the liquefaction process.

Supportive Processes

Solidification. Solids from S/L separation are cooled and further solidified so that they are suitable for use in gasification (hydrogen production). More solids are expected to be produced than are needed in gasification, and this excess will be disposed of as a solid waste.

Gas Purification. Gases from phase (gas) separation, hydrotreating, and hydrogen generation are purified by acid gas removal. Purified gases are sent to cryogenic separation for further purification.

Cryogenic Separation. Purified gas is taken from the preceding process and run through a series of cryogenic units. Products resulting from this process include synthetic natural gas, liquid petroleum gas, and light oils.

Sulfur Recovery. Acid gas from gas purification is converted to elemental sulfur in this process.

Hydrogen Generation. Some of the solidified mineral residue from solidification is used to generate hydrogen via gasification. The hydrogen is needed to increase the hydrogen/carbon ratio to the proportion required produce liquid fuels from coal:[2] The gasifier feed may consist of mineral residue only,[3,4] residue and coal,[2,5,7] or residue and oil[6].

Other Supportive Processes. Other processes which are needed, although they are not directly part of the liquefaction process, include:

- ammonia recovery
- phenol recovery
- oxygen generation
- steam generation
- product, by-product storage
- raw water treatment
- waste water treatment
- cooling towers
- power generation

5.3. Solid Wastes from SRC-II Process

Table 5.1 and Figure 5.2 summarize the sources and types of solid waste in SRC-II liquefaction (and preferred control technology, Table 5.1).

5.4. Assumptions Made in Modeling SRC-II Solid Wastes

The solid waste streams which are quantified in this module are limited to two, mineral residue and gasifier slag. In addition, estimates are made of the composition of the sulfur by-product and SRC product streams. Solid wastes from other sources are not quantified here (see individual solid waste descriptions).

The input coal is assumed to have been already subject to pretreating (cleaning) at Level 1 (as defined in Section 1). Any higher level of cleaning is fairly redundant, as the liquefaction itself can be considered a

Table 5.1
Summary of Solid Wastes Control Technology
Applicability to SRC Systems

Operation/Process	Solid Wastes Discharged	Preferred Control Technology Applications
Coal preparation	Refuse	(1) Landfill (2) Dumping (minefill)
Liquefaction	None	
Gas separation	None	
Fractionation	None	
Solids/liquid separation	Excess residue (SRC-II) or filter cake (SRC-I)	(1) Gasification to recovery energy content followed by disposal (landfill or minefill)
Hydrotreating	Spent catalyst	(1) Return to manufacturer for regeneration
Coal receiving and storage	None	
Water supply	Sludge	(1) Dewatering followed by landfilling
Water cooling	None	
Steam and power generation	Ash	(1) Landfill (2) Dumping (minefill)
Hydrogen generation	Ash or slag	(1) Landfill (2) Dumping (minefill)
Oxygen generation	None	
Acid gas removal	None	
Sulfur recovery	None	
Hydrogen/hydrocarbon recovery	None	
Ammonia recovery	None	
Phenol recovery	None	
Product/by-product storage	None	

Source: Reference 3.

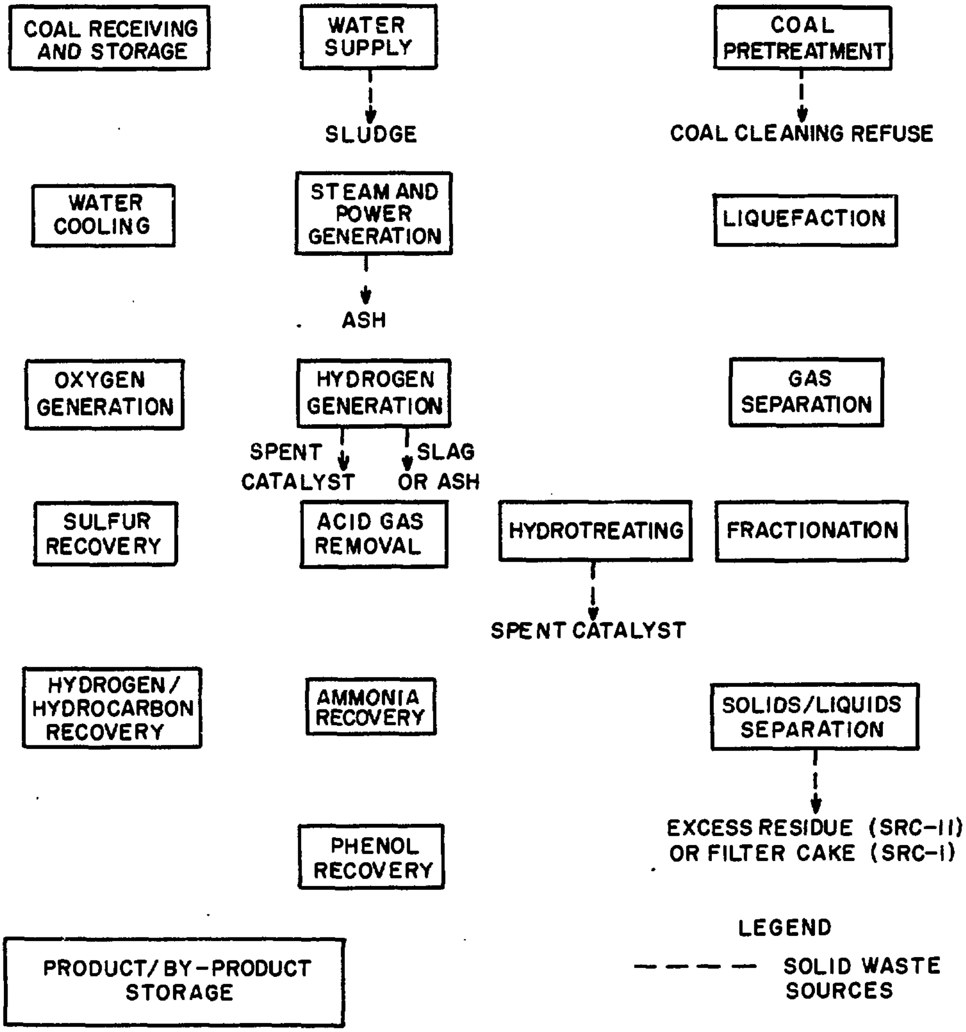

Figure 5.2 Sources of Solid Waste in SRC Systems (From Reference 7)

cleaning process. Part of the input coal is assumed to be sent directly to gasification, where it is combined with some of the mineral residue from the liquefaction process. This assumption requires no extra work for the module user; it is made because the trace metal data used herein are taken from Reference 7, which uses a residue/coal mixture in the gasifier. Failure to make the above assumption could therefore lead to trace metal mass balances greater than 100% due to the unaccounted input to the gasifier.

Since 100% mass balances may not, in reality, be obtained in the four output streams considered in this module (because of other waste and product streams), most elements have been normalized to achieve a 95% balance. While even this may be a large percentage, this assumption is made because (1) data for some elements led to mass balance greater than 100%, and (2) elements lost to other streams may be partially compensated for by addition from other inputs (e.g., solvents, catalysts, water).[6] See Appendix 5B for the description of trace element balance calculation.

5.5 Solid Wastes Not Quantified

Coal Cleaning Refuse. Coal dust and leachate from coal piles are not quantified here. Wastes from coal cleaning can be estimated elsewhere (see Section 1).

Ash from Steam and Power Generation. Solid wastes from generation can be estimated elsewhere (Section 2).

Sludge from Water Treatment. The composition of sludge from raw and waste water treatment is almost as dependent on the water composition as on the coal. Since the water characteristics can vary widely from site to site, these sludges can not be modeled in as general a way as this module intends.

Spent Catalysts from Hydrotreating and Hydrogen Generation. The lifetime of catalysts is inversely dependent upon operation time.[9] Therefore, purging of spent catalysts will be an intermittent and site specific process. This and the facts that (1) there is a wide variety of catalysts that may be used in the SRC-II process, and (2) some catalysts are regenerable (and therefore will not contribute to solid waste) makes modeling of spent catalysts impossible in this module.

5.6 SRC-II Liquefaction Module Description

The SRC-II module assumes constant removal rates of each of the input trace elements for each of the streams quantified, that is, a constant fraction of the total input element will be retained in the mineral residue, etc. (these constants will necessarily be different for each element and for each stream). Total quantities and major components of output streams are calculated as per Appendix 5A. The module is called with the following arguments:

1) total quantity of coal
2) input coal characteristics vector
3) output solid waste characteristics vectors

The input and output vectors each contain 50 elements. These elements are shown in Table 5.2. Since these vectors are constructed to be conformable to any of the solid waste modules which have been produced, there are presently some empty elements (48 to 50, not shown in Table 5.1) and some

Table 5.2
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium Sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

elements which are not applicable to this module, and as such are disregarded (set to 0) in the output vectors and omitted in the output printout.

Table 5.3 gives the coefficients which determine the amount of each trace element that goes to each solid waste stream.

Table 5.4 gives the equations which determine the total quantity of each stream and their major components (water, ash, sulfur and carbon).

It should be noted here that, given the data, some of these coefficients are little more than conjecture as to the "true" removal rates. Acquisition of more and better data is definitely indicated as a need for the future.

The appendices indicate how the choice of coefficients was made. Also in the appendices is more information on the computer module.

Table 5.3
Fractions (Coefficients) of Array Elements Going to Solid Waste Streams

Element	Mineral Residue	Gasifier Slag	Recovered Sulfur	SRC Product
Sb	0.728	0.219	0.002	0.001
As	0.842	0.102	0.003	0.003
Be	0.749	0.198	0.001	0.002
Cd	0.846	0.101	0.001	0.002
Cr	0.466	0.214	0.007	0.263
Cu	0.749	0.198	0.001	0.002
Fe	0.846	0.101	0.001	0.002
Pb	0.846	0.101	0.001	0.002
Mg	0.793	0.154	0.002	0.001
Mn	0.731	0.206	0.008	0.005
Hg	0.018	0.008	0.081	0.003
Ni	0.466	0.214	0.007	0.263
Se	0.838	0.092	0.019	0.001
Ag	0.846	0.101	0.001	0.002
Tl	0.846	0.101	0.001	0.002
Zn	0.731	0.206	0.008	0.005
U	0.793	0.154	0.002	0.001
Th	0.793	0.154	0.002	0.001
Ra^{226}	0.846	0.101	0.001	0.002
Ra^{228}	0.846	0.101	0.001	0.002
Pb^{210}	0.846	0.101	0.001	0.002

Table 5.4
Determination of Total Output and Major Components

Component	Mineral Residue	Gasifier Slag	Recovered Sulfur	SRC Product
Total quantity	$0.2\ I_c$	$0.083\ I_c$	$I_s-0.007\ O_{src}$	0.3
Sulfur	$0.02\ (I_s-0.007\ O_{src})$	$0.03\ (I_s-0.007\ O_{src})$	$0.95\ (I_s-0.007\ O_{src})$	0.00
Ash	$0.75\ (I_a-0.0015\ O_{src})$	$0.25\ (I_a-0.0015\ O_{src})$	-	0.00
Water	-	$0.4\ O_g$	-	
Carbon	$0.28\ O_r$	$0.001\ O_g$	-	0.87

I_x = total input amount of substance x
O_x = total output amount of substance x
c = coal.
src = SRC product.
r = mineral residue.
g = gasifier slag.
a = ash.
s = sulfur.
- = indicates zero amount contained.

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3. K.J. Shields, Environmental assessment report: Solvent-refined coal, Symp. Procs.: Environ. Aspects Fuel Conversion Technol. III, EPA-600/7-79-217, Sept. 1979.
4. C.R. Moxley, and D.K. Schmalzer, "Environmental Assessment of SRC-II - an Update", in Symp. Procs.: Environ. Aspects Fuel Conversion Technol. III, EPA-600/7-79-217, Sept. 1979.
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APPENDIX 5A

DETERMINATION OF OUTPUT STREAM CHARACTERISTICS: TOTAL QUANTITY, WATER, CARBON, SULFUR, ASH

5A.1 SRC Product

The total amount of SRC product seems to be fairly consistent relative to the amount of input (clean) coal, regardless of the coal characteristics:

Quantity Input Coal	Quantity SRC Product	Ratio	Source (Ref.)
20,408	6,080	0.2978	2
833,333	242,917	0.2915	8
10,000	2,920	0.2920	10

(Note: while units of measure may vary from source to source, the number of interest is the ratio, which is dimensionless. Therefore, the units involved will be disregarded.) The total product quantity will be assumed to be 30% of the quantity of input coal.

Similarly, the ash and sulfur contents of SRC product seem to be generally uniform regardless of the amounts contained in the input coal[9]. The ash content is in the range of .1 to .2%,[9-11,13] and sulfur content ranges from as low as .2%[7] to 1%,[10] with most estimates being from .5 to .8%[6,10,11,15] Therefore, the amounts of ash and sulfur, respectively, will be assumed to be .15% and .7% of the amount of SRC product.

Carbon content of the SRC product also seems constant, at about 87% of the total product[12]. It will be assumed that there is no water contained in the product.

5A.2 Recovered Sulfur

Most of the sulfur in the input coal is recovered from acid gases which are created during liquefaction and hydrogen generation[6]. Recovered sulfur will be assumed to be equal to 95% of the sulfur not retained in the SRC product. Of the remaining 5%, 2% is assumed lost to other (unquantified) streams and the other 3% is assumed to be retained in the mineral residue and gasifier slag.

Since there are no available data on recovered sulfur content of carbon, ash, and water, these components will be assumed to be nonexistent in the recovered sulfur. However, there may be some (fairly large) quantities of trace elements in the recovered sulfur[7]. Therefore, the total stream quantity is assumed to consist of sulfur (95%) and other elements (some of which are quantified in Appendix 5B).

While inorganic (pyritic) sulfur may not follow the same paths as organic sulfur in the liquefaction process,[10] because of lack of available data both forms of sulfur are assumed to be similarly distributed.

5A.3 Excess Mineral Residue

Of the total residue created in the SRC-II process, approximately 75% is excess (not directed to gasification for hydrogen generation[2,7]). This excess is approximately equal to 20% of the total input (clean) coal.

Quantity Input Coal	Quantity Excess M.R.	Ratio	Source (Ref.)
20,[illegible]	4,075	0.1997	2
19,994	4,203	0.2102	7

The carbon content is about 28%.[7] Since the residue has been solidified, water content is assumed to be 0.

Although there are no available data on the ash and sulfur content of the residue, most of what is not in the SRC product or recovered sulfur is expected to be retained in the residue. Therefore, 75% of the ash and 2% of the sulfur not retained in the SRC product are assumed to be in the residue.

5A.4 Gasifier Slag

The amount and character of gasifier slag is dependent on factors which may vary widely from site to site, such as gasifier feed composition and type of gasification process. However, some generalizations can be made about the resulting slag.

(1) Total (dry) slag can be estimated as about 5% of the input coal:

Quantity Input Coal	Quantity Gasifier Slag	Ratio	Source (Ref.)
20,408	1015.2	0.0497	2
20,000	1197.0	0.0599	5
19,944	922.8	0.0463	7
833,333	59400.0	0.0713	6

(2) The water:dry slag ratio is about 2:3.[2,7]

(3) Carbon is assumed to be a minor constituent (.1% of total dry slag) in the stream.

(4) While no data are available, ash and sulfur content can be assumed to be 25% (ash) and 1% (sulfur) of the respective total input amount which is not retained in the SRC product.

APPENDIX 5B

DETERMINATION OF OUTPUT STREAM CHARACTERISTICS: TRACE METALS

5B.1 General Discussion

There is a large void that needs to be filled in the realm of trace metal content of liquefaction output streams. Lack of complete and consistent data makes quantification of trace metal distribution an almost insurmountable task.

Reference 7 was the only source which contained enough data to estimate most trace metals for all output streams considered in this module. However, some of these data were estimates, rather than actual measured quantities. Several trace elements (Sb, Fe, Pb, U, Th) attained mass balances greater than 100 % in the four streams considered; others (e.g., Ni) had a large fraction unaccounted for. This over or under account of elements can be attributed to estimation techniques (for those not based on actual measurements), error in input coal and output stream measurements, loss of elements to other streams, and addition of elements from other sources.

The assumption was made to normalize all trace elements except mercury to 95 % of their input total, which allows for loss to other liquefaction output streams. Mercury is assumed to be largely lost in gaseous emissions because of its high volatility.[7] Elements for which there were only partial data were compared to other elements with complete data for distributional similarities, and the missing values were assumed to be the same as those of the similar element. Some elements which had missing data were treated on an individual basis.

5B.2 Trace Elements in Output Streams

Reference 7 is the basis for trace metal distributions. Estimations are based on the following quantities:

Q = total input coal: 19944 Mg/day -

m = total excess mineral residue: 4203 Mg/day -

g = total gasifier slag: 922.8 Mg/day -

r = total recovered sulfur: 443 Mg/day -

The trace element content of the "average U.S. coal" used is shown in table 5B.1. This coal was used as a basis for estimating the trace components of sulfur, SRC product, and slag. Partitioning factors (see below) were used to estimate trace elements in the mineral residue.

Table 5B.1
Trace Element Content of "Average U.S. Coal"

Element	Conc. (ppm).	Total Quantity (Tons)*	Element	Conc. (ppm).	Total Quantity (Tons)*
Sb	2.2	0.044	Hg	0.15	0.003
As	10.9	0.217	Ni	19.0	0.379
Be	1.4	0.028	Se	4.0	0.080
Cd	3.4	0.068	Ag	0.17	0.003
Cr	16.3	0.325	Tl	0.66	0.013
Cu	12.7	0.253	Zn	120.0	2.393
Fe	14,800.0	295.171	U	2.2	0.044
Pb	13.0	0.259	Th	4.5	0.09
Mg	1120.0	22.337	Ra	-	-
Mn	36.0	0.718			

Source: Reference 7, p. 175.
- Indicates data not available.
* Based on 19,944 tons of input coal.

Trace Metals in Mineral Residue. Estimated partitioning factors (Reference 7, p. 255) were given for the amount of trace elements in the mineral residue. The partitioning factor for each element, is defined as:

$$\frac{C_s}{C_i} ,$$

where,

C_x = the concentration of element C in stream x,

s = the output stream,

i = the input coal stream.

Since the total amount of an element in any stream x is

$$C_x \cdot t_x ,$$

where t_x = total quantity of stream x, then the proportion of that element which is retained in stream x is

$$\frac{C_x \cdot t_x}{C_i \cdot t_i} = \frac{C_x \cdot t_x}{C_i \cdot Q} .$$

This is simply the partitioning factor multiplied by the ratio of the output stream to the amount, Q, of input coal. In estimating the trace content of the residue, the minimum partitioning factors were used, as the average and maximum factors gave results that were greater than unity (i.e., a trace mass balance >100%). Even for the minimum factors, this occurred for two elements (Pb and U). Table 5B.2 gives the partitioning factors used and the mass proportion of elements retained in the residue.

Trace Metals in Other Output Streams. Trace content of other output streams is based upon either estimated (slag, sulfur) or measured (SRC product) concentrations. The proportions of the input elements captured in

Table 5B.2
Partitioning Factors and Proportion of Total Trace Elements Retained in Mineral Residue

Element	Partitioning Factor*	Proportion Retained**	Element	Partitioning Factor*	Proportion Retained**
Sb	4.3	0.906	Hg	0.031	0.007
As	4.0	0.843	Ni	0.4	0.084
Be	2.0	0.421	Se	3.6	0.759
Cd	1.6	0.337	Ag	-	-
Cr	1.0	0.211	Tl	-	-
Cu	2.1	0.443	Zn	2.0	0.421
Fe	4.6	0.969	U	6.6	1.391
Pb	5.2	1.096	Th	4.52	0.953
Mg	4.5	0.948	Ra	-	-
Mn	2.1	0.443			

Source: Reference 7, p. 255
- Indicates data not available.
* Minimum.
** Based on total proportion (Table 5B.1) and 4203:19944 residue to coal ratio.

these three streams are based on the total quantities of the streams as given above. The concentrations and proportions are shown in Table 5B.3.

5B.3 Trace Element Distribution Used in SRC-II Module

As mentioned above, no trace element achieved a 100% mass balance over the four output streams. Some elements had mass balances greater than 100%; others has less than 50% of the input amount accounted for. Some elements have missing data (partial or all).

Elements Having Complete Sets of Data. Elements with complete sets of data were normalized to have 95% of the input amount of that element accounted for, as explained above. This was accomplished by multiplying each of the four proportions by the normalization factor N,

Table 5B.3
Trace Elements in Slag, Recovered
Sulfur, and SRC Product

Element	Gasifier Slag Conc.*	 Proportion**	Recovered Sulfur Conc.*	 Proportion**	SRC Product Conc.*	 Proportion
Sb	13.0	0.273	0.2	0.002	0.003	0.001
As	24.0	0.102	1.7	0.003	0.006	0.003
Be	-	-	-	-	0.003	0.001
Cd	-	-	-	-	0.024	-
Cr	34.0	0.097	2.4	0.003	2.5	0.119
Cu	32.0	0.117	0.64	0.001	0.100	0.001
Fe	37000.0	0.116	740.0	0.001	62.0	0.002
Pb	20.0	0.071	-	-	0.007	0.001
Mg	-	-	290.0	0.006	2.1	0.001
Mn	97.0	0.125	8.6	0.005	0.790	0.003
Hg	0.0093	0.003	0.21	0.031	-	-
Ni	42.0	0.102	-	-	0.160	0.006
Se	7.2	0.083	3.0	0.017	0.003	0.001
Ag	-	-	-	-	-	-
Tl	-	-	-	-	0.007	0.005
Zn	180.0	0.069	-	-	0.100	0.005
U	-	-	-	-	0.007	0.001
Th	18.0	0.185	0.45	0.002	0.006	0.001
Ra	-	-	-	-	-	-

Source: Reference 7.
- Indicates data not available.
* All concentrations in ppm (wt.).
** Proportion of total element retained in stream.

$$N = \frac{.95}{\sum_i p_i} \qquad i = 1,2,3,4,$$

where the p_i are the calculated proportions of the element in the four streams (from Tables 5B.2 and 5B.3).

Elements with complete data are Sb, As, Cr, Cu, Fe, Mn, Se, and Th. The final distribution (after normalization) decided upon for these elements is given in Table 5B.3.

Elements with One or Two Missing Values. Elements with one or two missing values (except Hg, see below) were compared to elements with complete sets of data. If the distribution of the element with missing data seemed similar to one of the other elements, the former was assigned that complete distribution.

Elements with one or two missing data points and the comparable elements are

Missing Data	Complete Data
Be	Cu
Pb	Fe
Mg	Th
Ni	Cr
Zn	Mn
U	Th

Other Elements. Elements which have not been accounted for up until now include Cd, Hg, Ag, Tl, and Ra. These are assumed to be distributed as follows:

Hg is given an SRC product proportion of .001. It is then normalized to 11% of its input amount (89% unaccounted for[7]).

Cd, Ag, Tl, Ra are assigned the Fe distribution under the assumption that they are retained mostly in the residue (as are most trace elements[6,10]) The final proportional distribution of all trace elements are given in Table 5B.3.

APPENDIX 5C
DESCRIPTION OF COMPUTER MODULE

The SRC-II liquefaction solid waste module consists of one subroutine and a data file containing the fraction of the input components that are removed to the solid waste. The module is set into motion by a call to SRC-II:

Call SRCII (Q, COAL, MRES, SLAG, SUL, SRC)

where

Q = total mass in input coal

COAL = input coal characteristic vector

MRES = mineral residue from solidification output characteristic vector

SLAG = slag from gasifier output characteristic vector

SUL = by-product sulfur output characteristic vector

SRC = product SRC output characteristic vector

The subroutine first calculates the radium and lead-210 input quantities from the input uranium-238 and thorium-232 quantities if the former have not been supplied. See Section 7 for calculations of these quantities.

The subroutine calculates the characteristics of each output stream and prints them out (see Appendix 5D for sample output). The data file contains the coefficients of all elements that are removed at a constant rate and can be calculated by a simple multiplication. All elements in the input vector that are empty, are not applicable to this module, or are calculated other than by a single multiplication (e.g., sulfur, ash) have corresponding coefficient of zero.

All calculations (including empty and nonapplicable elements) are done through DO loops in the module. The water, ash, sulfur, carbon, and total solid waste elements are calculated separately.

The module prints out the input coal and output vectors (applicable elements only). If this printout is not desired at some future time, the printout section can simply be removed with no effect on the solid waste calculations. All vectors are returned to the calling program intact, including the input coal characteristics.

The data file is presently read in as "TAPE1".

APPENDIX 5D

COMPUTER CODE AND SAMPLE OUTPUT

This section sets out the computer code used for the SRC-II liquefaction module and the data file of coefficients, with a sample input and the resulting output. Table 5D.1 gives the coal characteristics used as input. The quantity of coal (Q) in the input is 100,000 tons.

At present the main program of the code is used only to set the input variables.

Table 5D.1
Input Characteristics of Coal

Element	Input Quantity (tons)
Ash	18700.00
Sulfur	3000.00
Antimony	0.07
Arsenic	2.70
Beryllium	0.50
Cadmium	0.125
Chromium	3.00
Copper	1.18
Iron	2700.00
Lead	1.14
Magnesium	118.00
Manganese	7.40
Mercury	0.017
Nickel	2.00
Selenium	0.02
Silver	0.01
Thallium	0.66
Zinc	1.69
Uranium	0.07
Thorium	0.66
Pyritic sulfur	1870.00
Carbon	64100.00
Btu	2.3×10^{12}

```
      PROGRAM CLL(TAPE1,OUTPUT,TAPE2=OUTPUT)
      DIMENSION COAL(50)
      REAL MRES(50),SLAG(50),SUL(50),SRC(50)
      Q=100000
      COAL(1)=18700.
      COAL(2)=3000.
      COAL(3)=.07
      COAL(4)=2.7
      COAL(5)=.5
      COAL(6)=.125
      COAL(7)=3.
      COAL(8)=1.18
      COAL(9)=2700
      COAL(10)=1.14
      COAL(11)=118.
      COAL(12)=7.4
      COAL(13)=.017
      COAL(14)=2.
      COAL(15)=.02
      COAL(16)=.01
      COAL(17)=.66
      COAL(18)=1.69
      COAL(19)=.07
      COAL(20)=.66
      DO 10 I=21,38
      COAL(I)=0.
   10 CONTINUE
      COAL(39)=1870.
      COAL(40)=64100
      COAL(41)=2.3E12
      DO 20 I=42,50
      COAL(I)=0.
   20 CONTINUE
      CALL SRCII(Q,COAL,MRES,SLAG,SUL,SRC)
      STOP
      END
```

```
      SUBROUTINE SRCII(Q,COAL,MRES,SLAG,SUL,SRC)
      DIMENSION COAL(50),MRES(50),SLAG(50),SUL(50),SRC(50)
      REAL MRES,MRESC(50),SLAGC(50),SULC(50),SRCC(50)
C   * COEFFICIENTS USED TO DETERMINE ELEMENTAL SPLIT BETWEEN
C   * OUTPUT WASTE AND PRODUCT STREAMS READ IN
      READ(1,1000)(MRESC(I),SLAGC(I),SULC(I),SRCC(I),I=1,50)
1000  FORMAT(F9.5,3F10.5)
C   * CALCULATION OF INPUT RA-226,RA-228 & PB-210 IF NOT GIVEN
      IF(COAL(21) .EQ. 0.)COAL(21)=3.38E-7*COAL(19)
      IF(COAL(22) .EQ. 0.)COAL(22)=4.01E-10*COAL(20)
      IF(COAL(23) .EQ. 0.)COAL(23)=4.37E-9*COAL(19)
C   * CALCULATION OF TRACE ELEMENT SPLIT BETWEEN OUTPUT STREAMS
      DO 10 I=3,24
      MRES(I)=MRESC(I)*COAL(I)
      SLAG(I)=SLAGC(I)*COAL(I)
      SUL(I)=SULC(I)*COAL(I)
      SRC(I)=SRCC(I)*COAL(I)
   10 CONTINUE
C   * NON-APPLICABLE ELEMENTS SET TO ZERO
      DO 20 I=26,50
      MRES(I)=0.
      SLAG(I)=0.
      SUL(I)=0.
      SRC(I)=0.
   20 CONTINUE
C   * CALCULATION OF TOTAL QUANTITY OF EACH OUTPUT STREAM
      MRES(25)=.2*Q
      SLAG(25)=.083*Q
      SRC(25)=.3*Q
      SUL(25)=COAL(2)-.007*SRC(25)
C   * CALCULATION OF ASH CONTENT OF EACH OUTPUT STREAM
      SRC(1)=.0015*SRC(25)
      MRES(1)=.75*(COAL(1)-SRC(1))
      SLAG(1)=.25*(COAL(1)-SRC(1))
         SUL(1)=0.
C   * CALCULATION OF SULFUR CONTENT OF EACH OUTPUT STREAM
      MRES(2)=.02*SUL(25)
      SLAG(2)=.01*SUL(25)
      SUL(2)=.95*SUL(25)
      SRC(2)=.007*SRC(25)
C   * CALCULATION OF INPUT PYRITIC SULFUR
      PSUL=COAL(39)/COAL(2)
C   * CALCULATION OF PYRITIC SULFUR CONTENT OF EACH OUTPUT STREAM
      MRES(39)=PSUL*MRES(2)
      SLAG(39)=PSUL*SLAG(2)
      SUL(39)=PSUL*SUL(2)
      SRC(39)=PSUL*SRC(2)
C   * CALCULATION OF WATER CONTENT OF GASIFIER SLAG
      SLAG(34)=.4*SLAG(25)
C   * CALCULATION OF CARBON CONTENT OF EACH OUTPUT STREAM
      MRES(40)=.28*MRES(25)
      SLAG(40)=.001*SLAG(25)
      SRC(40)=.87*SRC(25)
C
C
C        PRINT OUT OF DATA
C
C
      WRITE(2,2000)Q,COAL(1),MRES(1),SLAG(1),SUL(1),SRC(1),
     -COAL(2),MRES(2),SLAG(2),SUL(2),SRC(2),
     -COAL(3),MRES(3),SLAG(3),SUL(3),SRC(3),
     -COAL(4),MRES(4),SLAG(4),SUL(4),SRC(4)
2000  FORMAT(1H1,5X,*INPUT COAL:*2X,E12.5/1X,*ELEMENT*,T16,*INPUT COAL*,
```

```
     -T31,*MIN. RESID.*,T46,*GAS. SLAG*,T61,*SULFUR RECOVERY*,T81,*SRC*/
     -1X,105(*-*)/
     -1X,*ASH*,T16,E12.5,4(3X,E12.5)/
     -1X,*SULFUR*,T16,E12.5,4(3X,E12.5)/
     -1X,*ANTIMONY*,T16,E12.5,4(3X,E12.5)/
     -1X,*ARSENIC*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2001)COAL(5),MRES(5),SLAG(5),SUL(5),SRC(5),
     -COAL(6),MRES(6),SLAG(6),SUL(6),SRC(6),
     -COAL(7),MRES(7),SLAG(7),SUL(7),SRC(7),
     -COAL(8),MRES(8),SLAG(8),SUL(8),SRC(8)
2001  FORMAT(1X,*BERYLLIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*CADMIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*CHROMIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*COPPER*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2002)COAL(9),MRES(9),SLAG(9),SUL(9),SRC(9),
     -COAL(10),MRES(10),SLAG(10),SUL(10),SRC(10),
     -COAL(11),MRES(11),SLAG(11),SUL(11),SRC(11),
     -COAL(12),MRES(12),SLAG(12),SUL(12),SRC(12)
2002  FORMAT(1X,*IRON*,T16,E12.5,4(3X,E12.5)/
     -1X,*LEAD*,T16,E12.5,4(3X,E12.5)/
     -1X,*MAGNESIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*MANGANESE*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2003)COAL(13),MRES(13),SLAG(13),SUL(13),SRC(13)
     -,COAL(14),MRES(14),SLAG(14),SUL(14),SRC(14),
     -COAL(15),MRES(15),SLAG(15),SUL(15),SRC(15),
     -COAL(16),MRES(16),SLAG(16),SUL(16),SRC(16)
2003  FORMAT(1X,*MERCURY*,T16,E12.5,4(3X,E12.5)/
     -1X,*NICKEL*,T16,E12.5,4(3X,E12.5)/
     -1X,*SELENIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*SILVER*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2004)COAL(17),MRES(17),SLAG(17),SUL(17),SRC(17)
     -,COAL(18),MRES(18),SLAG(18),SUL(18),SRC(18),
     -COAL(19),MRES(19),SLAG(19),SUL(19),SRC(19),
     -COAL(20),MRES(20),SLAG(20),SUL(20),SRC(20)
2004  FORMAT(1X,*THALLIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*ZINC*,T16,E12.5,4(3X,E12.5)/
     -1X,*URANIUM*,T16,E12.5,4(3X,E12.5)/
     -1X,*THORIUM-232*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2005)COAL(21),MRES(21),SLAG(21),SUL(21),SRC(21)
     -,COAL(22),MRES(22),SLAG(22),SUL(22),SRC(22),
     -COAL(23),MRES(23),SLAG(23),SUL(23),SRC(23),
     -COAL(25),MRES(25),SLAG(25),SUL(25),SRC(25)
2005  FORMAT(1X,*RADIUM-226*,T16,E12.5,4(3X,E12.5)/
     -1X,*RADIUM-228*,T16,E12.5,4(3X,E12.5)/
     -1X,*LEAD-210*,T16,E12.5,4(3X,E12.5)/
     -1X,*TOTAL WASTE*,T16,E12.5,4(3X,E12.5))
      WRITE(2,2006)COAL(34),MRES(34),SLAG(34),SUL(34),SRC(34)
     -,COAL(39),MRES(39),SLAG(39),SUL(39),SRC(39),
     -COAL(40),MRES(40),SLAG(40),SUL(40),SRC(40)
2006  FORMAT(1X,*WATER*,T16,E12.5,4(3X,E12.5)/
     -1X,*PYRITIC SULFUR*,T16,E12.5,4(3X,E12.5)/
     -1X,*CARBON*,T16,E12.5,4(3X,E12.5)//)
      RETURN
      END
```

```
0.      0.      0.      0.
0.      0.      0.      0.
.728    .219    .002    .001
.842    .102    .003    .003
.749    .198    .001    .002
.846    .101    .001    .002
.466    .214    .007    .263
.749    .198    .001    .002
.846    .101    .001    .002
.846    .101    .001    .002
.793    .154    .002    .001
.731    .206    .008    .005
.018    .008    .081    .003
.466    .214    .007    .263
.838    .092    .019    .001
.846    .101    .001    .002
.846    .101    .001    .002
.731    .206    .008    .005
.793    .154    .002    .001
.793    .154    .002    .001
.846    .101    .001    .002
.846    .101    .001    .002
.846    .101    .001    .002
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
0.      0.      0.      0.
```

```
     INPUT COAL:     .10000E+06
ELEMENT       INPUT COAL     MIN. RESID.    GAS. SLAG      SULFUR RECOVERY     SRC
----------------------------------------------------------------------------------------
ASH             .18700E+05     .13991E+05     .46638E+04     0.              .45000E+02
SULFUR          .30000E+04     .55800E+02     .27900E+02      .26505E+04     .21000E+03
ANTIMONY        .70000E-01     .50960E-01     .15330E-01      .14000E-03     .70000E-04
ARSENIC         .27000E+01     .22734E+01     .27540E+00      .81000E-02     .81000E-02
BERYLLIUM       .50000E+00     .37450E+00     .99000E-01      .50000E-03     .10000E-02
CADMIUM         .12500E+00     .10575E+00     .12625E-01      .12500E-03     .25000E-03
CHROMIUM        .30000E+01     .13980E+01     .64200E+00      .21000E-01     .78900E+00
COPPER          .11800E+01     .88382E+00     .23364E+00      .11800E-02     .23600E-02
IRON            .27000E+04     .22842E+04     .27270E+03      .27000E+01     .54000E+01
LEAD            .11400E+01     .96444E+00     .11514E+00      .11400E-02     .22800E-02
MAGNESIUM       .11800E+03     .93574E+02     .18172E+02      .23600E+00     .11800E+00
MANGANESE       .74000E+01     .54094E+01     .15244E+01      .59200E-01     .37000E-01
MERCURY         .17000E-01     .30600E-03     .13600E-03      .13770E-02     .51000E-04
NICKEL          .20000E+01     .93200E+00     .42800E+00      .14000E-01     .52600E+00
SELENIUM        .20000E-01     .16760E-01     .18400E-02      .38000E-03     .20000E-04
SILVER          .10000E-01     .84600E-02     .10100E-02      .10000E-04     .20000E-04
THALLIUM        .66000E+00     .55836E+00     .66660E-01      .66000E-03     .13200E-02
ZINC            .16900E+01     .12354E+01     .34814E+00      .13520E-01     .84500E-02
URANIUM         .70000E-01     .55510E-01     .10780E-01      .14000E-03     .70000E-04
THORIUM-232     .66000E+00     .52338E+00     .10164E+00      .13200E-02     .66000E-03
RADIUM-226      .23660E-07     .20016E-07     .23897E-08      .23660E-10     .47320E-10
RADIUM-228      .26466E-09     .22390E-09     .26731E-10      .26466E-12     .52932E-12
LEAD-210        .30590E-09     .25879E-09     .30896E-10      .30590E-12     .61180E-12
TOTAL WASTE    0.              .20000E+05     .83000E+04      .27900E+04     .30000E+05
WATER          0.             0.              .33200E+04     0.             0.
PYRITIC SULFUR  .18700E+04     .34782E+02     .17391E+02      .16521E+04     .13090E+03
CARBON          .64100E+05     .56000E+04     .83000E+01     0.              .26100E+05
```

6 SOLID WASTE MODULE FOR OIL SHALE RETORTING

6.1 Introduction

As a possible substitute for petroleum, the reserves of oil shale have attracted widespread attention. Commercial interest in the extraction and processing of oil shale has existed for several decades. A viable oil shale industry has been "about to start" several times this century but each time economic, technical, political, or legal roadblocks have postponed actual development. Recently the impetus to develop domestic energy sources has prompted new interest in oil shale activities. This has also led to increased concern about the environmental impacts which might be associated with large-scale extraction and processing operations. Of particular concern are the possible impacts of solid waste disposal. About 80% of the mined shale remains after retorting, giving rise to huge quantities of waste. Further, the spent shale occupies a much greater volume than the raw material.

6.2 Oil Extraction from Oil Shale

The oil in oil shale is contained in kerogen, a solid, powdery, largely insoluble organic substance. The oil is obtained by heating which breaks the chemical network holding the heavy kerogen molecules together and "cracks" the individual large molecules into smaller molecules. This releases a liquid hydrocarbon mixture, some combustible gases, and a coke-like residue.

The conventional way of recovering the oil is to mine the shale and put it through the heating process aboveground. A more recent method is to break up the shale while it is still in the ground and heat it in place (in situ).

Conventional Recovery. Conventional recovery consists of four basic steps: mining the shale, crushing it to the proper size for the retort vessel, retorting the shale to release the oil, and refining the oil to bring it up to a high-quality product. The shale is mined either underground or on the surface by conventional methods. It is then crushed and reduced to the size required for the particular heating method to be used.

The crushed shale is fed into a closed retorting vessel and heated to very high temperatures - between 800° and 1000°F - to decompose the kerogen. The various retorting processes apply heat to the shale in different ways.

The oily vapor produced as the kerogen decomposes during retorting is condensed to form the raw shale oil. This oil has a high nitrogen content as well as appreciable quantities of sulfur and oxygen.

At the refinery, raw shale oil is upgraded to remove the nitrogen, sulfur, and oxygen. This is done by reacting the oil with hydrogen so that it becomes a synthetic crude oil that is essentially the same as high grade conventional crude oil.

In Situ Recovery. In "true" in situ processing, the in place shale is fractured using explosives to create void spaces in the shale. The shale is ignited and a combustible gas pumped in. The hot combustion gases circulate along the pathways in the fractured shale heating it to retorting temperature. The vapors produced condense to a liquid in a sump at the base of the shale area and is pumped to the surface.

In a "modified" version of the in situ recovery, about 30% of the lower portion of the shale bed is first mined by conventional methods. This portion is retorted aboveground.

6.3 Processes Used in the Module

At present, there are no full-scale oil shale operations. The module, therefore, will compute the solid waste produced from the two conventional processes closest to commercialization - TOSCO II and Paraho (direct mode). In both cases, full-scale plants have been designed and it is on these plans that the solid waste module is based.

The basic distinction between the processes is the method of heat transfer. In the Paraho process (Figure 6.1), the heat for retorting is supplied by combustion of residual carbonaceous material in denuded shale in the lower portion of the retorting vessel. The hot combustion gases flow upwards through the shale liberating shale oil vapors at a temperature of approximately 900°F from the fresh shale entering the upper section of the vessel. In the proposed commercial Paraho process, the raw shale oil is condensed and stored without any further on-site processing. In the TOSCO II process (Figure 6.2), preheated shale is fed to a horizontal rotating retort (pyrolysis drum) where a charge of hot ceramic balls contacts the raw shale, raising its temperature to 900°F. The organic matter in the shale is converted to shale oil vapor which is withdrawn from the retorting vessel. In the proposed commercial TOSCO II process the raw shale oil is upgraded onsite.

A true in situ process produces no waste requiring disposal. The modified in situ plant has 20 to 30% of the shale mined by conventional methods. This can be retorted using conventional methods. Therefore, for the modified in situ plant the model can be run using an input quantity of raw shale which reflects the initial 20 to 30%.

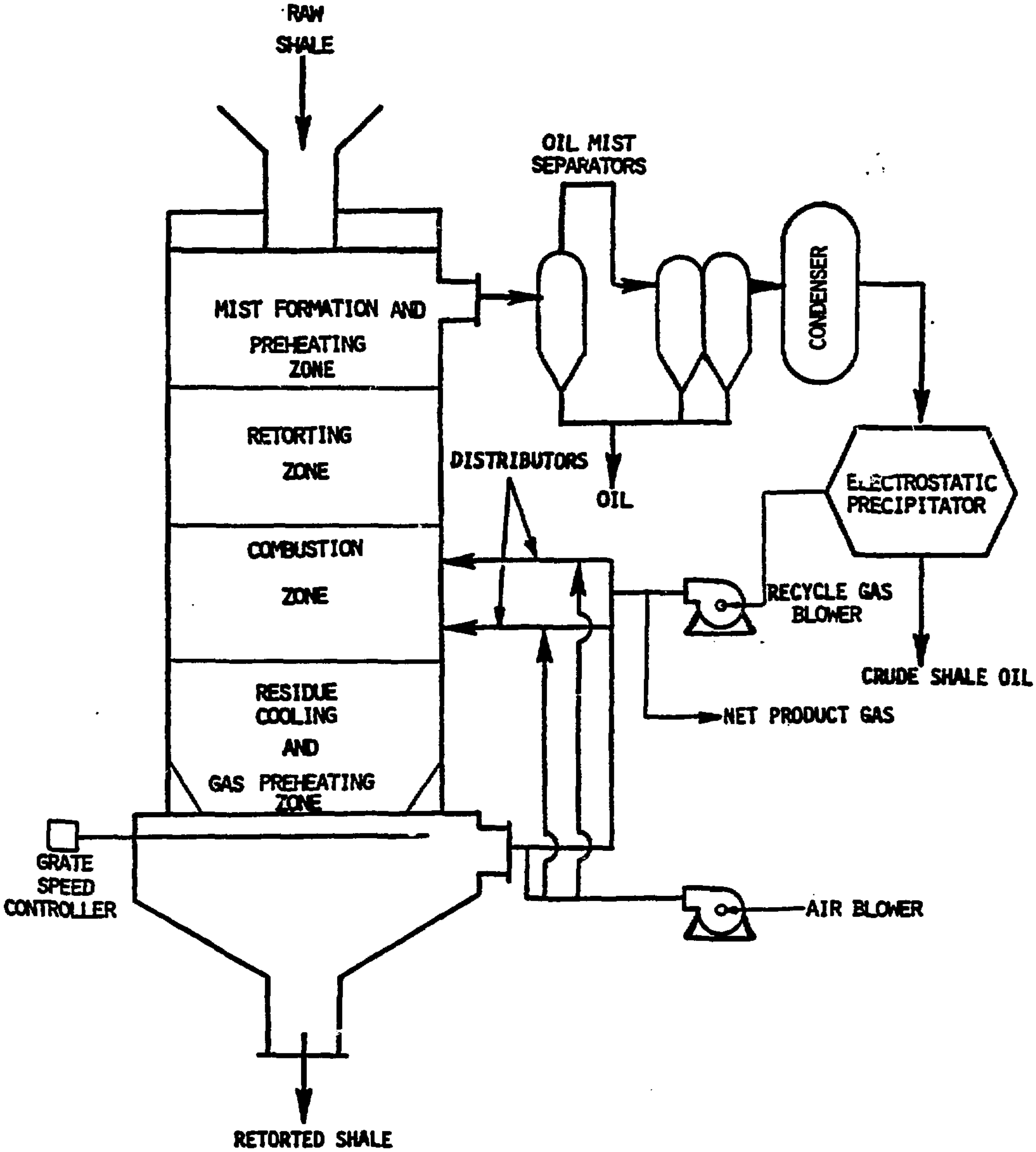

Figure 6.1 Paraho process. (From Reference 2.)

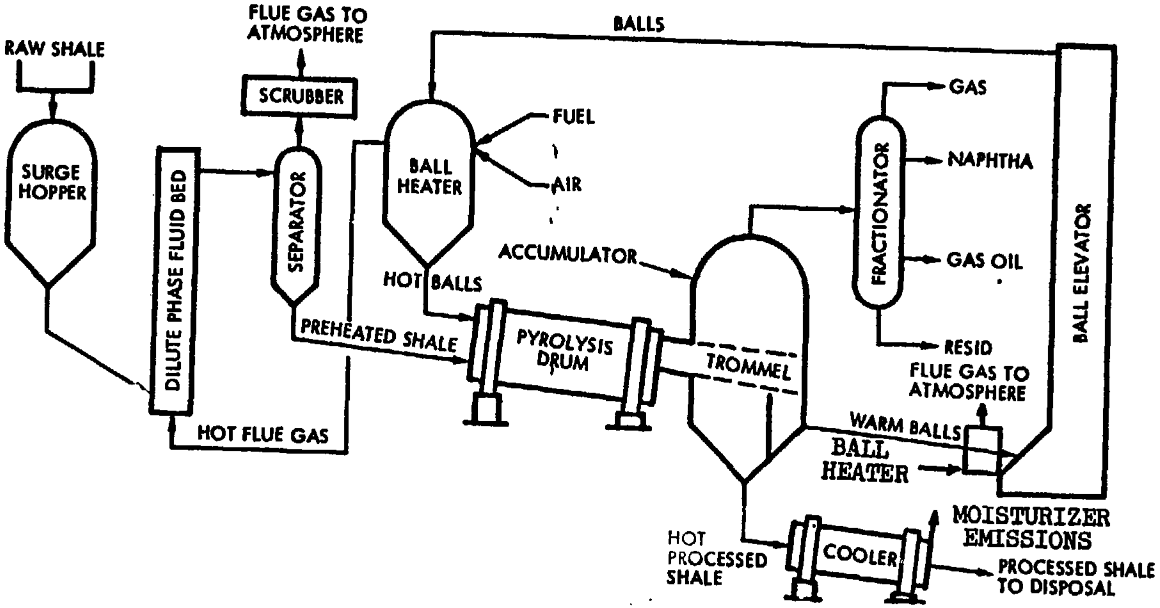

Figure 6.2 TOSCO II process. (From Reference 2.)

6.4 Solid Waste Produced by Oil Shale Recovery

The major quantities of solid waste are from the crushing and retorting operations.

In the TOSCO II process there is no minimum size for the shale particles entering the retort and so the only waste comes from the collection of fugitive particulate matter. For the Paraho process, the minimum particle size is 3/8-in.[1] The <3/8-in. fines can either be disposed of as waste or briquetted and sent to the retorts.

In both cases the composition of the waste is, of course, essentially the same as that of the raw shale.

By far the largest quantity of waste comes from the spent shale. In the module this also includes particulate matter which is collected during the retorting process.

The character of the waste depends on the retorting process used. Spent shale from the TOSCO II process contains about 5% residual carbonaceous material, whereas in the Paraho process the spent shale is partially "burned" after pyrolysis of oil shale kerogen and contains only 2% organic carbon. The composition of Paraho spent shale is similar to Portland cement. It also has some cement-like properties which help to create stable disposal piles. The TOSCO II waste consists of very fine crystalline particles. There are no cement-like properties, and this could lead to problems with pile stability and leaching.

Table 6.1 lists the other wastes produced by oil shale processing. Only the quantity of recovered arsenic will be given in the module. The bio-oxidation sludge is as dependent on the water composition as on the process and can vary greatly, making it impossible to model in this type of

Table 6.1
Solid Waste Other than Spent Shale

Waste Description	Source	Process	Disposition
Bio-oxidation sludge	Process condensate	Paraho	Spent shale
	Domestic waste	TOSCO II	Spent shale
Sulfur	Sulfur recovery	Paraho	Sell as by-product
		TOSCO II	Sell as by-product
API separator sludge	Oil/water separator	Paraho	Return to retort
		TOSCO II	Return to retort
Shale oil coke	Refinery	TOSCO II	Sell as by-product
Spent catalysts	Refinery	TOSCO II	Ship to manufacturer for recovery
Arsenic	Refinery	TOSCO II	Ship to hazardous waste disposal off-site

module. The oil coke and sulfur are to be sold and therefore do not constitute a waste product. The present plans also assume that the catalysts will be shipped to the manufacturer for recovery. Even if they were to be disposed of on site, the intermittent nature of their disposal makes it impossible to model in this module.

6.5 Oil Shale Module Description

The module assumes constant removal rates for each of the input trace elements for each of the streams quantified. That is, a constant fraction of the total input elements will be retained in the spent shale, etc. (these constants will necessarily be different for each element and for each stream).

The input to the module is the quantity of raw oil shale and its composition in terms of sulfur, carbon, and trace elements and an integer value (1 to 4) to indicate which retorting process is to be employed (Paraho, TOSCO II, or modified in situ using either Paraho or TOSCO II).

Figure 6.3 gives an overall view of the module. For both processes the sequence is the same but the coefficients vary. The module first computes the amount of shale which is lost during crushing operations and appears as solid waste. The remainder of the shale goes to retorting. Here the total quantities of solid waste and product oil are calculated. The amounts of the trace elements in the spent shale and oil are computed. There are also gas and condensate water streams in the retorting process, but since the module is concerned with solid waste these are not included. To simply give the approximate quantity of the elements in the initial gas stream would not be very meaningful, since the gas undergoes a number of cleaning steps, and a fraction is recycled to provide heat for the retorting process. Therefore, the final composition of the gas vented to the atmosphere would be very different. For the TOSCO II process the amount of recovered arsenic is also given.

The module is called by the main program with the following arguments:

Total input quantity of oil shale

Input vector of oil shale characteristics

Output vector of raw shale waste composition

Output vector of spent shale composition

Output vector of crude oil composition

Output vector of recovered arsenic

Type of process to be employed. Integer number: 1 - Paraho; 2 - TOSCO II; 3 - modified in situ using Paraho; and 4 - modified in situ using TOSCO II.

Grade of oil shale (gal/ton)

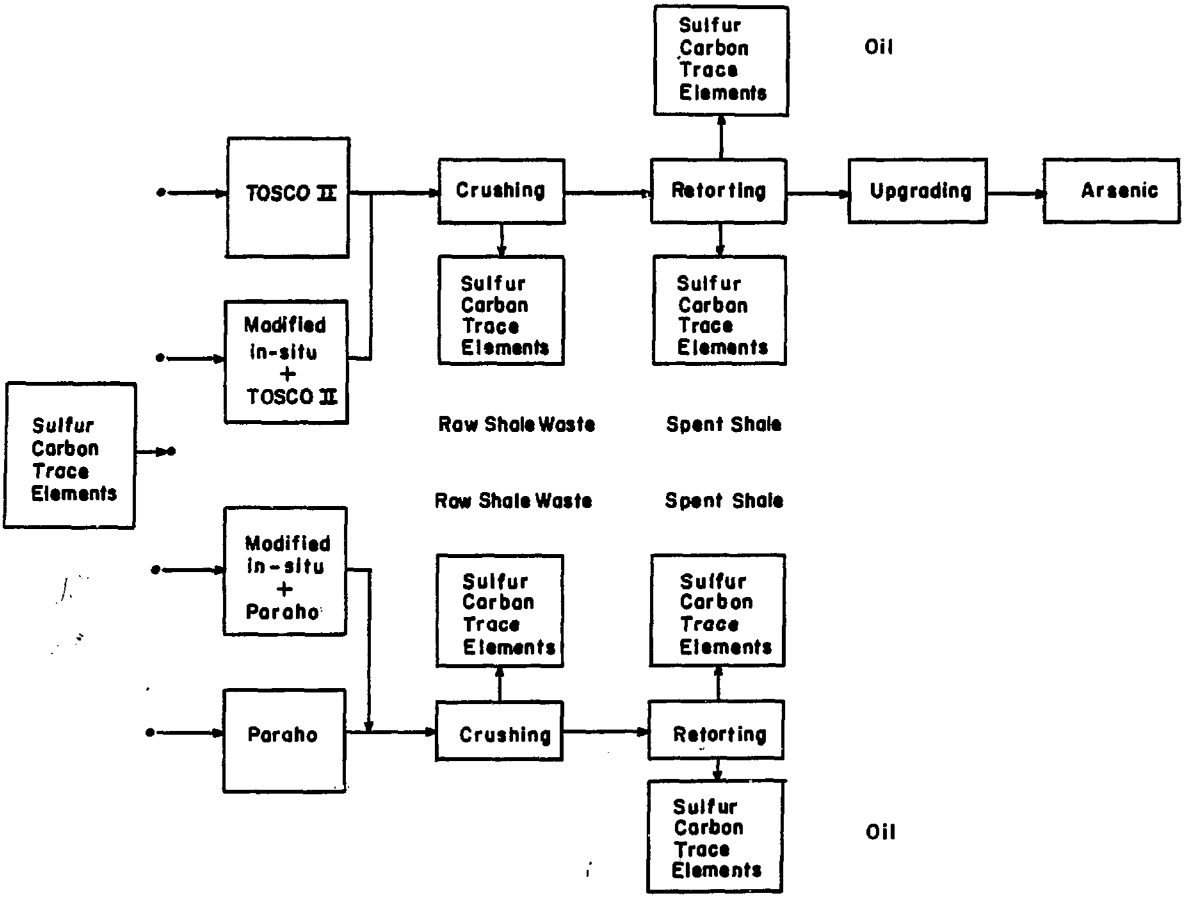

Figure 6.3 Overall oil shale module design.

The input and output vectors each contains 50 elements (Table 6.2). Since these vectors are constructed to be conformable to any of the solid waste modules which have been produced, there are presently some empty elements (48 to 50, not shown) and some elements which are not applicable to this module and as such are disregarded (set to 0) in the output vectors and omitted in the output printout.

Tables 6.3 and 6.4 give the equations for the total quantities of waste and product oil and their major components, for the TOSCO II and Paraho processes respectively. The coefficient for the total quantity of spent shale is used to calculate the dry weight. The output vector elements give the disposal weight, i.e., dry weight plus water.

Table 6.5 gives the coefficients which determine the amount of each trace element in the spent shale and oil. In addition, for trace elements in the raw shale waste stream the coefficients are the same as for the total waste, i.e., 0.007 for TOSCO II and 0.05 for Paraho. The reduced amounts are then used as input to the retorting process.

Because there are few good data available on the fate of the trace elements during retorting, many of the figures are very rough estimates. They will need to be revised when better data become available.

It should also be noted that in a number of cases less than a 100% of an element is accounted for. This is because the remainder is found in the gas and water condensate streams which are not considered in the module.

The appendices give more information on the source of the coefficients and details of the computer code.

Table 6.2
Elements

Number	Type	Number	Type
1	Ash	24	Hydrocarbons
2	Sulfur (S)	25	Total solid waste
3	Antimony (Sb)	26	Unreacted limestone
4	Arsenic (As)	27	Calcium sulfite
5	Beryllium (Be)	28	Calcium sulfate
6	Cadmium (Cd)	29	Soda ash
7	Chromium (Cr)	30	Magnesium sulfite
8	Copper (Cu)	31	Magnesium oxide
9	Iron (Fe)	32	Sodium bisulfite
10	Lead (Pb)	33	Sodium sulfite
11	Magnesium (Mg)	34	Water
12	Manganese (Mn)	35	Sulfur dioxide
13	Mercury (Hg)	36	Nitrous oxides
14	Nickel (Ni)	37	Carbon monoxide
15	Selenium (Se)	38	Methane
16	Silver (Ag)	39	Pyritic sulfur
17	Thallium (Tl)	40	Carbon
18	Zinc (Zn)	41	Btu
19	Uranium-238 (U)	42	Carbon dioxide
20	Thorium-232 (Th)	43	Sodium bicarbonate
21	Radium-226 (Ra)	44	Sodium carbonate
22	Radium-228 (Ra)	45	Sodium sulfate
23	Lead-210 (Pb)	46	Calcium carbonate
		47	Calcium oxide

Table 6.3
Coefficients for Total Output and Major Components for TOSCO II

Components	Raw Shale Waste	Spent Shale	Oil	Arsenic Waste
Total quantity (dry)	0.007 I_{os}	0.81 R_{os}	0.004 $R_{os} x OG$	0.0075 $R_a x 5.0$
Sulfur	0.007 I_s	0.79 R_s	0.08 R_s	
Carbon	0.007 I_c	0.2 R_c	0.7 R_c	
Water		0.14 O_{ss}		
Arsenic				0.0075 R_a

I_x = Total input amount of substance x.
O_x = Total output amount of substance x.
R_x = Total amount of substance x into the retort (I_x - 0.007 I_x).
os = Oil shale.
s = Sulfur.
c = Carbon.
ss = Spent shale.
OG = Grade of oil shale (gal/ton raw oil shale).
a = Arsenic.

Table 6.4
Coefficients for Total Output and Major Components for Paraho

Components	Raw Shale Waste	Spent Shale	Oil
Total quantity (dry)	0.05 I_{os}	0.8 R_{os}	0.004 R_{os} x 0.92 OG
Sulfur	0.05 I_s	0.79 R_s	0.08 R_s
Carbon	0.05 I_c	0.08 R_c	0.7 R_c
Water		0.05 O_{ss}	

I_x = Total input amount of substance x.
O_x = Total output amount of substance.
R_x = Total amount of substance x into retort (I_x - 0.05 I_x).
os = Oil shale.
s = Sulfur.
c = Carbon.
ss = Spent Shale.
OG = Grade of oil shale (gal/ton raw oil shale).

Table 6.5
Fractional Split of Trace Elements between Spent Shale and Oil

Element	Spent Shale	Oil
Antimony	99.9	0.1
Arsenic	85.0	5.0
Beryllium	100.0	0.0
Cadmium	100.0	0.0
Chromium	99.8	0.2
Copper	99.9	0.1
Iron	99.9	0.1
Lead	99.9	0.1
Magnesium	99.9	0.1
Manganese	99.9	0.1
Mercury (Paraho)	4.8	5.2
Mercury (TOSCO II)	1.4	6.7
Nickel	99.1	0.9
Selenium	89.9	0.1
Silver	99.9	0.1
Thallium	99.9	0.1
Zinc	99.6	0.4
Uranium	99.9	0.1
Thorium	99.9	0.1
Radium	99.9	0.1

REFERENCES

1. U.S. Department of Energy, Environmental Control Costs for Oil Shale Processes, DOE/EV-0055, Washington, DC, 1979.

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3. T.A. Henderson (ed.), Synthetic Fuels Data Handbook, Cameron Engineers, Inc., Denver, CO, 1975.

4. Bureau of Standards, Thermal Properties of Petroleum Products, Miscellaneous Publication No. 97, U.S. Department of Commerce, Washington, DC, 1929.

5. A.D. Schendrikar and G.B. Faudel, Distribution of trace metals during oil shale retorting, Environ. Sci. and Technol., 12, 332, 1978.

APPENDIX 6A

CALCULATION OF MAJOR COMPONENTS OF OUTPUT STREAMS

6A.1 Raw Shale and Spent Shale Waste

The figures are based on the actual quantities of waste that are expected from a commercial size plant as given in the present plant designs[1,2].

The waste from crushing is greater for the Paraho process because some fines are included.

For both processes the spent shale from retorting includes particulate matter collected from the retorting process and from the wetting of the spent shale prior to disposal.

6A.2 Water

In both cases, the spent shale is moistened prior to disposal. Since the waste from the two processes has differing characteristics, different amounts of water are required. Again the quantities are based on plant designs[1].

6A.3 Crude Oil Production

In order to be compatible with the rest of the output elements, the quantity of oil product is given in tons.

The grade of oil shale in terms of gallons of oil per ton of shale is given as an input. It is determined with a Fisher Assay, which uses a bench retorting system to determine the quantity of oil in a sample of shale. The TOSCO II process should recover 100% of the Fisher Assay; however, in the Paraho process the expected yield is only 92%. The oil production is converted from gallons to tons using a density of 7.7 lb/gal[3,4].

6A.4 Sulfur

The distribution of sulfur comes from a Fisher Assay[3]. The distribution may be different in commercial plants. Using this distribution does give reasonable agreement with some figures given in References 1 and 2.

6A.5 Carbon

The module only considers the fate of the organic carbon. The only complete data available are for the total kerogen. It is therefore assumed that the carbon has the same distribution. The split again comes from a Fisher Assay,[3] which gives a large organic residue remaining in the shale after pyrolysis. In commercial operations, depending on the process, this residue may be partially burned after pyrolysis, e.g., the Paraho process. In the TOSCO II process the organic residue is not burned; it was therefore decided to use the split given by the Fisher Assay. This does give reasonable results for the amount of carbon left in the spent shale for the TOSCO II process[2]. In the Paraho process the residue is partially burned and the spent shale contains only 2% carbon as opposed to 5% for the TOSCO II process[2]. It was assumed that the same amount of carbon appeared in the oil as for TOSCO II, but the amount in the spent shale was reduced. The remainder is assumed to be in the gas as combustion products.

6A.6 Recovered Arsenic

In the TOSCO II process arsenic is recovered during upgrading procedures. The amount is from the plant design and it is assumed that arsenic constitutes 20% of the total waste[1].

APPENDIX 6B

TRACE METAL COMPOSITION OF OUTPUT STREAMS

Very few data are available on the trace metals in oil shale and their fate during retorting. In many cases the coefficients are little more than conjectures.

The only reported results on the mass balance of elements around a retort are for the following elements[5]:

As
Be
Cd
Cr
Cu
Pb
Mn
Ni
Se
Zn

These results were based on a Fisher Assay and concentrations were measured only in the oil, spent shale, and condensate water. No measurements were made of the gaseous phase. In most cases this does not appear to matter; except for As and Se, mass balances close to unity were achieved and it would appear that virtually all elements remain with the spent shale. This is also the conclusion given in Reference 1. From Reference 1 it is assumed that 10% of the As and Se appear in the gas. This is in agreement with the unrecovered portion shown in Reference 5. The mass balances given in Reference 5 were therefore recalculated assuming that 10% of these elements escaped with the gas.

The route of Hg in a commercial plant is highly speculative. Although it is assumed that virtually all of the Hg initially appears in the gas, it may later condense and appear in the spent shale, oil, recovered sulfur, and spent catalysts[1]. The amount of Hg in the spent shale and gas could vary by 90%.[1]

At present, in the module it is assumed that the majority of the Hg is in the gas. However, if evidence becomes available that more Hg is found elsewhere the figures will have to be revised.

There are no data for the remaining elements.

Sb
Fe
Mg
Ag
Tl
U
Th
Ra

Since these elements are not very volatile, it is assumed that they remain with the spent shale.

APPENDIX 6C

DESCRIPTION OF COMPUTER MODULE

The oil shale solid waste module consists of one subroutine and a data file containing the fraction of the input components that are removed to the solid waste. The module is set in motion by a call to SHALE:

CALL SHALE (QS, OILSH, RAWSH, SPENTS, OIL, ARSNC, OGRADE, IMETH),

where

QS = total mass of input shale
OILSH = input oil shale characteristic vector
RAWSH = raw shale output characteristic vector
SPENTS = spent shale output characteristic vector
OIL = oil output characteristic vector
ARSNC = arsenic output characteristic vector
OGRADE = input grade of oil shale (gal/ton)
IMETH = process type:
  1 = Paraho
  2 = TOSCO II
  3 = modified in situ + Paraho
  4 = modified in situ + TOSCO II

The subroutine calculates the solid waste characteristics of each waste stream and prints them out (see Appendix 6D for sample output). The data file contains the coefficients of all elements that are removed at a constant rate for both processes and can be calculated by a simple multiplication. All elements in the input vector that are empty, are not applicable to this module, are calculated differently for the two processes, or are calculated other than by a single multiplication (e.g., water and total solid wastes) have corresponding coefficients of zero.

All calculations (including dummy calculations for empty and nonapplicable elements) are done through DO loops in the module. The water, sulfur, carbon, arsenic, and mercury elements are calculated separately for each process.

The module prints out the input oil shale, output oil and waste vectors (applicable elements only). If this printout is not desired at some future time, the printout section can simply be removed with no effect on the solid waste calculations. All vectors are returned to the calling program intact, including the input oil shale characteristics.

The data file is presently read in as "TAPE1".

APPENDIX 6D

COMPUTER CODE AND SAMPLE OUTPUT

This section sets out the computer code used for the oil shale module and the data file of coefficients, with a sample input and the resulting output. Table 6D.1 gives the oil shale characteristics used as input. The other input variables used were as follows:

Quantity of oil shale (QS) = 100,000 tons

Grade of oil shale (OGRADE) = 35 gal/ton

Process (IMETH) = 2 (TOSCO II)

At present the main program of the code is used only to set the input variables.

Table 6D.1
Input Characteristics of Oil Shale

Element	Input Quantity (tons)
Sulfur	700.00
Antimony	0.15
Arsenic	4.00
Beryllium	0.10
Cadmium	0.10
Chromium	3.50
Copper	4.00
Iron	4720.00
Lead	2.50
Magnesium	1550.00
Manganese	25.00
Mercury	0.02
Nickel	2.50
Selenium	0.15
Silver	0.01
Thallium	0.01
Zinc	7.00
Uranium	0.37
Thorium	1.20
Pyritic sulfur	400.00
Carbon	10465.00

```
      PROGRAM CLL(TAPE1,OUTPUT,TAPE2=OUTPUT)
      DIMENSION OILSH(50)
      REAL RAWSH(50),SPENTS(50),OIL(50),ARSNC(50)
      QS=100000
      OILSH(1)=0.
      OILSH(2)=700.
      OILSH(3)=.15
      OILSH(4)=4.0
      OILSH(5)=.1
      OILSH(6)=.1
      OILSH(7)=3.5
      OILSH(8)=4.0
      OILSH(9)=4720
      OILSH(10)=2.5
      OILSH(11)=1550
      OILSH(12)=25.
      OILSH(13)=.02
      OILSH(14)=2.5
      OILSH(15)=.15
      OILSH(16)=.01
      OILSH(17)=.01
      OILSH(18)=7.0
      OILSH(19)=.37
      OILSH(20)=1.2
      DO 10 I=21,38
      OILSH(I)=0.
   10 CONTINUE
      OILSH(39)=400.
      OILSH(40)=10465
      OILSH(41)=0.
      DO 20 I=42,50
      OILSH(I)=0.
   20 CONTINUE
          OGRADE=29.
          IMETH=1
      CALL SHALE(QS,OILSH,RAWSH,SPENTS,OIL,ARSNC,OGRADE,IMETH)
      STOP
      END
```

```
      SUBROUTINE SHALE(QS,OILSH,RAWSH,SPENTS,OIL,ARSNC,OGRADE,IMETH)
      DIMENSION OILSH(50),RAWSH(50),SPENTS(50),OIL(50),ARSNC(50)
      REAL RAWSH,RAWSHC(50),SPENTSC(50),OILC(50),ARSNCC(50)
C   * COEFFICENTS USED TO DETERMINE ELEMENTAL SPLIT BETWEEN
C   * PRODUCT AND WASTE STREAMS READ IN
      READ(1,1000)(RAWSHC(I),SPENTSC(I),OILC(I),ARSNCC(I),I=1,50)
1000  FORMAT(F9.5,3F10.5)
C   * CALCULATION OF INPUT RA-226,RA-228 & PB-210 IF NOT GIVEN
      IF(OILSH(21) .EQ. 0.)OILSH(21)=3.38E-7*OILSH(19)
      IF(OILSH(22) .EQ. 0.)OILSH(22)=4.01E-10*OILSH(20)
      IF(OILSH(23) .EQ. 0.)OILSH(23)=4.37E-9*OILSH(19)
      DO 10 I=1,50
C   * TOSCOII PROCESS .7% CRUSHING LOSS AS SOLID WASTE
C   * PARAHO PROCESS 5% CRUSHING LOSS AS SOLID WASTE
      IF(IMETH .EQ. 2 .OR. IMETH .EQ. 4)RAWSHC(I)=.007
      IF(IMETH .EQ. 1 .OR. IMETH .EQ. 3)RAWSHC(I)=.05
C   * CALCULATION OF ELEMENTAL SPLIT BETWEEN OUTPUT STREAMS
      RAWSH(I)=RAWSHC(I)*OILSH(I)
      SPENTS(I)=SPENTSC(I)*(OILSH(I)-RAWSH(I))
      OIL(I)=OILC(I)*(OILSH(I)-RAWSH(I))
      ARSNC(I)=ARSNCC(I)*(OILSH(I)-RAWSH(I))
   10 CONTINUE
      IF(IMETH .EQ. 1 .OR. IMETH .EQ. 3)GO TO 101
C   * FOLLOWING CALCULATIONS FOR TOSCOII PROCESS
C   * CALCULATION OF TOTAL QUANTITY OF OUTPUT STREAMS
      RAWSH(25)=.007*QS
      SPENTS(25)=.81*(QS-RAWSH(25))
      OIL(25)=.004*OGRADE*(QS-RAWSH(25))
      ARSNC(25)=5.*.0075*(OILSH(4)-RAWSH(4))
C   * CALCULATION OF SULFUR IN SPENT SHALE AND OIL
      SPENTS(2)=.79*(OILSH(2)-RAWSH(2))
      OIL(2)=.08*(OILSH(2)-RAWSH(2))
C   * CALCULATION OF PYRITIC SULFUR IN SPENT SHALE AND OIL
      SPENTS(39)=.79*(OILSH(39)-RAWSH(39))
      OIL(39)=.08*(OILSH(39)-RAWSH(39))
C   * CALCULATION OF CARBON IN SPENT SHALE AND OIL
      SPENTS(40)=.2*(OILSH(40)-RAWSH(40))
      OIL(40)=.7*(OILSH(40)-RAWSH(40))
C   * CALCULATION OF ARSENIC IN ARSENIC WASTE
      ARSNC(4)=.0075*(OILSH(4)-RAWSH(4))
C   * CALCULATION OF MERCURY IN SPENT SHALE AND OIL
      SPENTS(13)=.014*(OILSH(13)-RAWSH(13))
      OIL(13)=.067*(OILSH(13)-RAWSH(13))
C   * CALCULATION OF WATER CONTENT AND TOTAL QUANTITY OF SPENT SHALE
      SPENTS(34)=.14*SPENTS(25)
      SPENTS(25)=SPENTS(25)+SPENTS(34)
      GO TO 12
C   * FOLLOWING CALCULATIONS FOR PARAHO PROCESS
C   * CALCULATION OF TOTAL QUANTITY OF OUTPUT STREAMS
  101 RAWSH(25)=.05*QS
      SPENTS(25)=.8*(QS-RAWSH(25))
      OIL(25)=.004*.92*OGRADE*(QS-RAWSH(25))
C   * CALCULATION OF SULFUR & PYRITIC SULFUR CONTENT OF SPENT
C   * SHALE AND OIL
      SPENTS(2)=.79*(OILSH(2)-RAWSH(2))
      SPENTS(39)=.79*(OILSH(39)-RAWSH(39))
```

```
     OIL(2)=.08*(OILSH(2)-RAWSH(2))
     OIL(39)=.08*(OILSH(39)-RAWSH(39))
C   * CALCULATION OF CARBON CONTENT OF SPENT SHALE AND OIL
     SPENTS(40)=.08*(OILSH(40)-RAWSH(40))
     OIL(40)=.7*(OILSH(40)-RAWSH(40))
C   * CALCULATION OF WATER CONTENT AND TOTAL AMOUNT OF SPENT SHALE
     SPENTS(34)=.05*SPENTS(25)
     SPENTS(25)=SPENTS(25)+SPENTS(34)
C   * CALCULATION OF MERCURY CONTENT OF SPENT SHALE AND OIL
     SPENTS(13)=.048*(OILSH(13)-RAWSH(13))
     OIL(13)=.052*(OILSH(13)-RAWSH(13))
C
C
C        PRINT OUT OF DATA
C
C
  12 WRITE(2,2000)QS,OILSH(1),RAWSH(1),SPENTS(1),OIL(1),ARSNC(1),
    -OILSH(2),RAWSH(2),SPENTS(2),OIL(2),ARSNC(2),
    -OILSH(3),RAWSH(3),SPENTS(3),OIL(3),ARSNC(3),
    -OILSH(4)',RAWSH(4),SPENTS(4),OIL(4),ARSNC(4)
2000 FORMAT(1H1,5X,*INPUT OILSH:*2X,E12.5/1X,*ELEMENT*,T16,
    -*INPUT OILSHALE*,
    -T31,*RAW SHALE*,T46,*SPENT SHALE*,T61,*OIL*,T81,*ARSENIC*,/
    -1X,105(*-*)/
    -1X,*ASH*,T16,E12.5,4(3X,E12.5)/
    -1X,*SULFUR*,T16,E12.5,4(3X,E12.5)/
    -1X,*ANTIMONY*,T16,E12.5,4(3X,E12.5)/
    -1X,*ARSENIC*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2001)OILSH(5),RAWSH(5),SPENTS(5),OIL(5),ARSNC(5),
    -OILSH(6),RAWSH(6),SPENTS(6),OIL(6),ARSNC(6),
    -OILSH(7),RAWSH(7),SPENTS(7),OIL(7),ARSNC(7),
    -OILSH(8),RAWSH(8),SPENTS(8),OIL(8),ARSNC(8)
2001 FORMAT(1X,*BERYLLIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*CADMIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*CHROMIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*COPPER*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2002)OILSH(9),RAWSH(9),SPENTS(9),OIL(9),ARSNC(9),
    -OILSH(10),RAWSH(10),SPENTS(10),OIL(10),ARSNC(10),
    -OILSH(11),RAWSH(11),SPENTS(11),OIL(11),ARSNC(11),
    -OILSH(12),RAWSH(12),SPENTS(12),OIL(12),ARSNC(12)
2002 FORMAT(1X,*IRON*,T16,E12.5,4(3X,E12.5)/
    -1X,*LEAD*,T16,E12.5,4(3X,E12.5)/
    -1X,*MAGNESIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*MANGANESE*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2003)OILSH(13),RAWSH(13),SPENTS(13),OIL(13),ARSNC(13)
    -,OILSH(14),RAWSH(14),SPENTS(14),OIL(14),ARSNC(14),
    -OILSH(15),RAWSH(15),SPENTS(15),OIL(15),ARSNC(15),
    -OILSH(16),RAWSH(16),SPENTS(16),OIL(16),ARSNC(16)
2003 FORMAT(1X,*MERCURY*,T16,E12.5,4(3X,E12.5)/
    -1X,*NICKEL*,T16,E12.5,4(3X,E12.5)/
    -1X,*SELENIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*SILVER*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2004)OILSH(17),RAWSH(17),SPENTS(17),OIL(17),ARSNC(17)
    -,OILSH(18),RAWSH(18),SPENTS(18),OIL(18),ARSNC(18),
    -OILSH(19),RAWSH(19),SPENTS(19),OIL(19),ARSNC(19),
    -OILSH(20),RAWSH(20),SPENTS(20),OIL(20),ARSNC(20)
```

```
2004 FORMAT(1X,*THALLIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*ZINC*,T16,E12.5,4(3X,E12.5)/
    -1X,*URANIUM*,T16,E12.5,4(3X,E12.5)/
    -1X,*THORIUM-232*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2005)OILSH(21),RAWSH(21),SPENTS(21),OIL(21),ARSNC(21)
    -,OILSH(22),RAWSH(22),SPENTS(22),OIL(22),ARSNC(22),
    -OILSH(23),RAWSH(23),SPENTS(23),OIL(23),ARSNC(23),
    -OILSH(25),RAWSH(25),SPENTS(25),OIL(25),ARSNC(25)
2005 FORMAT(1X,*RADIUM-226*,T16,E12.5,4(3X,E12.5)/
    -1X,*RAOIUM-228*,T16,E12.5,4(3X,E12.5)/
    -1X,*LEAD-210*,T16,E12.5,4(3X,E12.5)/
    -1X,*TOTAL WASTE*,T16,E12.5,4(3X,E12.5))
     WRITE(2,2006)OILSH(34),RAWSH(34),SPENTS(34),OIL(34),ARSNC(34)
    -,OILSH(39),RAWSH(39),SPENTS(39),OIL(39),ARSNC(39),
    -OILSH(40),RAWSH(40),SPENTS(40),OIL(40),ARSNC(40)
2006 FORMAT(1X,*WATER*,T16,E12.5,4(3X,E12.5)/
    -1X,*PYRITIC SULFUR*,T16,E12.5,4(3X,E12.5)/
    -1X,*CARBON*,T16,E12.5,4(3X,E12.5)//)
         END
```

```
0.        0.        0.        0.
0.        0.        0.        0.
0.        .999      .001      0.
0.        .85       .05       0.
0.        1.        0.        0.
0.        1.        0.        0.
0.        .998      .002      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        0.        0.        0.
0.        .991      .009      0.
0.        .899      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .996      .004      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        .999      .001      0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
0.        0.        0.        0.
```

```
     INPUT OILSH:     .10000E+06
ELEMENT          INPUT OILSHALE RAW SHALE        SPENT SHALE     OIL                 ARSENIC
--------------------------------------------------------------------------------------------
ASH              0.               0.               0.               0.               0.
SULFUR            .70000E+03       .35000E+02       .52535E+03       .53200E+02      0.
ANTIMONY          .15000E+00       .75000E-02       .14236E+00       .14250E-03      0.
ARSENIC           .40000E+01       .20000E+00       .32300E+01       .19000E+00      0.
BERYLLIUM         .10000E+00       .50000E-02       .95000E-01      0.               0.
CADMIUM           .10000E+00       .50000E-02.      .95000E-01      0.               0.
CHROMIUM          .35000E+01       .17500E+00       .33184E+01       .66500E-02      0.
COPPER            .40000E+01       .20000E+00       .37962E+01       .38000E-02      0.
IRON              .47200E+04       .23600E+03       .44795E+04       .44840E+01      0.
LEAD              .25000E+01       .12500E+00       .23726E+01       .23750E-02      0.
MAGNESIUM         .15500E+04       .77500E+02       .14710E+04       .14725E+01      0.
MANGANESE         .25000E+02       .12500E+01       .23726E+02       .23750E-01      0.
MERCURY           .20000E-01       .10000E-02       .91200E-03       .98800E-03      0.
NICKEL            .25000E+01       .12500E+00       .23536E+01       .21375E-01      0.
SELENIUM          .15000E+00       .75000E-02       .12811E+00       .14250E-03      0.
SILVER            .10000E-01       .50000E-03       .94905E-02       .95000E-05      0.
THALLIUM          .10000E-01       .50000E-03       .94905E-02       .95000E-05      0.
ZINC              .70000E+01       .35000E+00       .66234E+01       .26600E-01      0.
URANIUM           .37000E+00       .18500E-01       .35115E+00       .35150E-03      0.
THORIUM-232       .12000E+01       .60000E-01       .11389E+01       .11400E-02      0.
RADIUM-226        .12506E-06       .62530E-08       .11869E-06       .11881E-09      0.
RADIUM-228        .48120E-09       .24060E-10       .45668E-09       .45714E-12      0.
LEAD-210          .16169E-08       .80845E-10       .15345E-08       .15361E-11      0.
TOTAL WASTE      0.                .50000E+04       .79800E+05       .10138E+05      0.
WATER            0.               0.                .38000E+04      0.               0.
PYRITIC SULFUR    .40000E+03       .20000E+02       .30020E+03       .30400E+02      0.
CARBON            .10465E+05       .52325E+03       .79534E+03       .69592E+04      0.
```

7 RADIONUCLIDES

7.1 Radionuclides Included in the Solid Waste Modules

Radionuclides are important constituents of coal and oil shale and it was decided that a number should be included in the solid waste modules. The reasons for including the following radionuclides are given below.

Radionuclides Produced by Cosmic Rays. The longest-lived radionuclide, Be^{10}, has a half-life of only $2.5x10^6$ years,[1] and can thus be ignored. C^{14} is discussed separately below.

Carbon-14. C^{14} is a radionuclide produced in the upper atmosphere by cosmic rays (and also in nuclear power plants). When plants die, their C^{14} is in equilibrium with that in air. However, since its half-life is 5730 years, there is very little left in coal.

Primordial radionuclides. The most important of these radionuclides, potassium-40, has a half-life of $1.26x10^9$ years and is a significant contributor to natural radiological dose.[1] Rubidium-87 is also worth consideration. However, because of the very long half-life of primordial radionuclides and the fact that their concentration in coal is no greater than in the earth's crust, there is no reason to treat them separately from the element as a whole in the data base and transport equations. They can be broken out at any time using the known amount per mass of the total element.

Radioactive isotopes of potassium and rubidium always occur as a constant fraction of the total element; there is no relative body buildup of the radioactive isotopes and hence no changes in health effects.

Since potassium and rubidium are not being considered as trace elements, it was decided there was no reason to include their radioactive isotopes.

Naturally Occurring Decay Chains. There are three naturally occurring decay chains: (1) uranium series headed by U^{238}, (2) actinium series headed by U^{235}, and (3) thorium series headed by Th^{232}. The main sequences of nuclides for each of these are given in Tables 7.1 to 7.3.

Table 7.1
Uranium Series
Main Decay Chain
(Minor Side Chains Excluded)

Nuclide	Half-LIfe		Decay Mode	Branching Ratio, %
U^{238}	4.5×10^{9}	y	α	100
Th^{234}	24.10	d	β^-	100
Pa^{234}	1.175	m	β^-	100
U^{234}	2.5×10^{5}	y	α	100
Th^{230}	8.0×10^{4}	y	α	100
Ra^{226}	1.6×10^{3}	y	α	100
Rn^{222}	3.82	d	α	100
Po^{218}	3.05	m	α	99+
Pb^{214}	26.8	m	β^-	100
Bi^{214}	19.7	m	β^-	99+
Po^{214}	164.0	μs	α	100
Pb^{210}	22.3	y	β^-	99+
Bi^{210}	5.01	d	β^-	99+
Po^{210}	138.38	d	α	100
Pb^{206}	stable			

Source: Reference 2.

Table 7.2
Actinium Series
Main Decay Chain
(Minor Side Chains Excluded)

Nuclide	Half-LIfe	Decay Mode	Branching Ratio, %
U^{235}	7.0x10^{8} y	α	100
Th^{231}	25.52 h	β^-	100
Pa^{231}	3.3x10^{4} y	α	100
Ac^{227}	21.773 y	β^-	98.6
Th^{227}	18.718 d	α	100
Ra^{223}	11.435 d	α	100
Rn^{219}	3.96 s	α	100
Po^{215}	1.78 ms	α	99+
Pb^{211}	36.1 m	β^-	100
Bi^{211}	2.15 m	α	99.7
Ti^{207}	4.77 m	β^-	100
Pb^{207}	stable		

Source: Reference 2.

Table 7.3
Thorium Series
Main Decay Chain
(Minor Side Chains Excluded)

Nuclide	Half-LIfe	Decay Mode	Branching Ratio, %
Th^{232}	1.41x10^{10} y	α	100
Ra^{228}	5.76 y	β^-	100
Ac^{228}	6.13 h	β^-	100
Th^{228}	1.91 y	α	100
Ra^{224}	3.66 d	α	100
Rn^{220}	55.6 s	α	100
Po^{216}	0.15 s	α	100
Pb^{212}	10.64 h	β^-	100
Bi^{212}	60.60 m	β^- (1)	64
		α (2)	36
(1)Po^{212}	0.3 s	α	100
(2)Tl^{208}	3.053 m	β^-	100
Pb^{208}	stable		

Source: Reference 2.

If the series is in secular equilibrium, the activities (divided by branching fraction to that daughter) of all daughters are the same. Thus, given the amount of any one nuclide, the amounts of the others can be calculated knowing the half-life and atomic weight:

$$m(2) = m(1) \frac{T(2)\ A(2)}{T(1)\ A(1)}$$

where

m = mass

A = atomic weight

T = half-life

In this case of the three decay chains, specifying the U (natural) and Th contents would be sufficient information. (Natural uranium is 99.3% U^{238} and 0.7% U^{235}). These are exactly the data given in the USGS coal data base.

Unfortunately, there are forces acting towards disequilibrium as the coal lies in its bed, during combustion, and in solid waste piles. For example, radium may be preferentially leached from waste piles. Thus, in theory, one must consider individually three dozen odd major nuclides and many minor ones. However, in practice, one may consider only those daughters with long half-lives without compromising the accuracy of an assessment significantly. A list of these radionuclides is given below.

U	Uranium	Pb^{210}	Lead
Th	Thorium	Rn^{222}	Radon
Ra^{228}	Radium	Pa^{231}	Protactinium
Ra^{226}		Ac^{227}	Actinium

While release of radon may be important when the disposal of the waste is considered, its release rate from waste piles can be calculated from the amount of radium.

Inclusion of protactinium and actinium are a refinement of U^{235} decay chain effects which constitutes only 1% of the total uranium. Since data are not readily available for these elements, they will not be considered.

7.2 Mass Calculations of Radium and Lead-210

The mass of radium-226 and lead-210 in the input coal, oil shale and limestone can be calculated from the uranium-238 and that of radium-238 from the thorium-232, using the following equations and assumptions.

7.2.1 When Assuming Secular Equilibrium

The relevant principle here is that the branching ratio-weighted activity of any nuclide in a chain is equal to any other. Then, since the activity is proportional to M/AT,

$$M_b = M_a \frac{BR_b}{BR_a} \frac{A_b}{A_a} \frac{T_b}{T_a} ,$$

where

M = mass

BR = branching ratio to the nuclide

A = atomic weight

T = half-life

7.2.2 When Relative Activities Available

$$M_b = r(b/a)\ M_a \frac{A_b}{A_a} \frac{T_b}{T_a} \ ,$$

where

r(b/a) is the ratio of activity "b" to activity "a".

7.2.3 Special Case: $BR_x = 1$

Since all of the decays flow through Ra^{226}, Pb^{210}, and Ra^{228} in their decay chains, BR=1. Thus we can use the equation

$$M_b = r(b/a)\ M_a \frac{A_b}{A_a} \frac{T_b}{T_a} \ ,$$

with the understanding that r(b/a) = 1 in secular equilibrium.

Substituting in the following values results in the coefficients given below:

Nuclide	A	T (years)	AT
U^{238}	238	4.47×10^{9}	1.06×10^{12}
Ra^{226}	226	1.60×10^{3}	3.62×10^{5}
Pb^{210}	210	22.3	4.68×10^{3}
Th^{232}	232	1.41×10^{10}	3.27×10^{12}
Ra^{228}	228	5.76	1.31×10^{3}

$M_{Ra}{}^{226} = 3.38\times10^{-7}\ 8(Ra^{226}/U^{238})\ M_{U\text{-}nat}$

$M_{Pb}{}^{210} = 4.37\times10^{-9}\ r(Pb^{210}/U^{238})\ M_{U\text{-}nat}$

$M_{Ra}{}^{228} = 4.01\times10^{-10}\ r(Ra^{228}/Th^{232})\ M_{Th}$

The conversions include the fact that U^{238}/U-natural is 0.993 and Th-natural is essentially all Th^{232}.

Until further data become available, secular equilibrium and therefore a ratio of activity of 1 is assumed.