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INTRODUCTION

The U.S. Department of Energy (DOE) is investigating CO_2 recovery from fossil-fuel cycles as a greenhouse gas mitigation strategy. Recognizing this, we used life-cycle analysis tools to compare two integrated gasification combined-cycle (IGCC) plant designs based on the Shell entrained-flow gasifier. One option, called the "co-product case," uses high-sulfur Illinois #6 coal to produce electricity and hydrogen (H_2) as energy carriers. At the same time, 90% of the carbon dioxide (CO_2) is recovered for disposal in geological storage or for use, such as enhanced-oil recovery (EOR). The second option, called the "base case," is a conventional IGCC power plant releasing CO_2 by combustion of the synthesis gas in a gas turbine. The life-cycle analysis task has been aided by use of LCAdvantage[TM]. Process design has been aided by the use of the ASPEN© simulation for critical design areas. Special attention is paid to the transport issues for the CO_2 product, because transportation technology is a determinant of product specifications, which affect plant design. Separating and purifying the H_2 for fuel cell use should yield an impressive gain in overall process efficiency, offsetting the losses in efficiency from recovery and compression of CO_2 to supercritical conditions.

OBJECTIVE - LOW GREENHOUSE IMPACT GASIFICATION CYCLES

Plant Design Basis
The Shell (entrained-flow) coal gasification system has been selected as the basis for the co-product plant. The energy and environmental performances of the co-product plant are

compared with those of a base-case plant that also uses the Shell gasification technology but produces only electricity as a salable product. The base-case IGCC plant and the co-product plant are substantially different in design. The most significant common elements are the use of the Shell gasifier and the consumption of the same amount and type of coal. Principal features and differences are summarized in Table 1.

Shell Gasification-Based Combined Cycle with Hydrogen, Electricity and CO_2
Figure 1 presents an overview of some of the critical process areas of the co-product plant, clarifying the differences noted in Table 1. The plant is conceptually divided into five main plant areas. Each area consists of a set of related processes. The processes in turn are composed of equipment or unit operations and process streams connect these. A two-digit taxonomy has been adapted for consistency in referring to these plant elements. The first digit designates the plant area, while the second designates the process. Table 2 presents a summary and comparison of the plant performance for a Base Case integrated gasification combined-cycle plant (IGCC), the proposed plant and an IEA study.

Coal Mining, Coal Washing, Transportation and Preparation
Coal characteristics and the impacts of the coal-preparation circuit appear in Table 3. The mining, coal-sizing and washing circuits are considered integral to the design of the gasification system. An underground mine near Seeser Illinois supplies Illinois #6 coal using long-wall continuous mining feeds 4,967 tons/day of raw coal to a washing circuit employing a jig, two crushers, three screens, a centrifuge and a thickener. This provides a more uniform product in the 5 x 1.5 in. size range with considerable reduction of the ash and modest reductions of pyritic sulfur. Employing this washing circuit shows a considerable advantage in reducing the tonnage of coal shipped by rail to the plant because the mining operation brings in roof and floor material. Calculations show that 81% of the energy from the raw coal reaches the product. At the same time, only 65% of the original tonnage of coal needs to be transported and handled. We have assumed that cleaning plant refuse is returned to the mine. The water use is 11.3 gallons/ton of raw coal, and the electricity use is 7 kWh/ton of raw coal. As a consequence of shaking and abrasion, coal losses of 0.05%/100 miles of rail transport are included.

10-Raw Materials Preparation

A material balance for the major process streams appear in Tables 4.1-4.3. The front end of the plant is nearly unchanged through Area 20. Hence, the gasification; heat recovery; particulate removal; and COS hydrolysis follow the base-case performance as originally modeled by Wally Shelton, EG&G.

11-Coal Preparation: After delivery by unit train a pulverizing circuit prepares the coal for transport into the gasifier using hot inert nitrogen from the 12-Air Separation Unit. In pulverizing and transporting the coal, further drying takes place so that a net 2,977 tons/day of coal is feed to the gasifier. The coal is combined with steam in transport, but does not mix with oxygen until the gasifier.

12-Air Separation Unit (ASU): A cryogenic unit provides 2,558 tons/day of oxygen feed to the gasifier at 95% purity. Nitrogen at 2.1% and Argon at 2.9% are inert diluents that carry through the rest of the cycle.

13-Water treatment: Conditioning of raw water for feed to the boiler and gasifier are essential so that steam service maintains a high efficiency. The process consumes 87 tons/day of steam as a chemical reagent in the gasification while a further 160 tons/day is consumed in the 31- Shift block. Sour water and blow-down streams also are treated in the plant.

20-Gasification

21-Gasification: The Shell gasifier receives the dry coal feed into an oxygen-blown, entrained-flow slagging unit that operates at 367 psi. The gasifier exit conditions are controlled by a feedback system on the oxygen so that the exit temperature before quench is 2,500 F. One critical design decision is to employ a gas recycle stream from 24-COS Hydrolysis block rather than quenching the hot raw gas with a water spray. This significantly reduces the water treatment from this system as contrasted with other commercial oxygen-blown, entrained-flow gasifiers.

22-Heat Recovery and 23-Particulate Removal: The raw gas product has considerable enthalpy that is converted to steam and employed for power generation.   Because of the dust loading coming off the gasifier, the design of these sections present some particularly challenging materials of construction, fabrication, and heat-transfer issues. A dust-free raw product gas at 450 F with a minor pressure drop is delivered for 24-COS Hydrolysis treatment.

24-COS Hydrolysis: This section converts the COS produced in gasification to H_2S. It is included in the 20-Gasification process block because nearly 30% of the product stream is recycled to the raw gas exiting the gasifier to serve as a quench. Any HCl and nearly all the ammonia entering with the raw gas stream is captured in this section and reports to the sour water.

30-Gas Conversion

31-Shift Reaction: The shift reaction uses 160 tons/day of steam to convert CO in the gasifier product stream to CO_2 and Hydrogen. The reaction takes place in two beds of sulfur-tolerant shift catalyst. The first bed of lower activity catalyst yields a 76% conversion. The temperature of the shift product form the first stage must be returned to 452 F so that 98% conversion in the second bed is feasible. Because these reactions are exothermic, cooling of the shift product from the two stages provides an additional 4.9 MW of power in the 32-Heat Recovery process block.

40-Gas Separation and Purification

41-H_2S Recovery: Glycol-based absorber-stripper processes for H_2S and CO_2 are commonly employed for gas clean up. Commercial systems generally employ an optimized mixture of five or more glycols, however, the vendors of these systems have provided warnings that the physical properties data for their mixtures are not well-simulated using data in the open literature. The current ASPEN 10.2 simulation solely employs tetra-Ethylene Glycol di-Methyl Ether ($C_{10}H_{22}O5$) as a surrogate for the commercial mixture.   Using this physical solvent and a 25 molar % water mix, more than 98% of the H_2S is captured in this section. This H_2S is

recovered for treatment in the 44-Claus process block that will yield a sulfur product. The next stage of glycol-based scrubbing recovers a very high fraction of residual H_2S so that a product specification of 10 ppm H_2S in the turbine fuel is met. While the glycols are more selective for H_2S than for CO_2, nearly 60% of the CO_2 is captured here.

42-CO_2 Recovery: A second glycol-based absorber-stripper system is employed for polishing so that a total of 90% of the CO_2 is captured for recovery and pipeline transport. After drying, 6,612 tons/day of CO_2 is compressed to 2,100 psi and transported from the plant using a super-critical pipeline. Commercial experience shows that other species such as H_2S are permissible in co-mixtures with CO_2 for injection into underground reservoirs. An effort to determine whether this co-mixture could be adequately simulated is reported in a later paper.

43-Pressure Swing Adsorption: This approach is commonly used in the purification of hydrogen. It is a semi-continuous process, which yields 357 tons/day of a very high purity hydrogen product, with some minor Argon dilution. The blow down product from this system has a significant heating value and is employed as a turbine fuel for power generation.

50-Power Generation

51-Combustion Turbine; 52-Heat Recovery Steam Generator; 53-Steam Cycle: These process areas are configured so that after the gas turbine (61.95 MW) the Heat recovery Steam Generator employs three steam pressures.

Additional output from steam cycle with incorporation of raw gas cooling: 86.63 MW
Low pressure turbine output from shift system heat: 4.9 MW
Total power generation: 153.48 MW.
Internal power requirements: -77.4 MW

Looking at the power balance over the entire plant, it is clear that most of the power is being exported over the fence as hydrogen.

APPROACH TO LIFE-CYCLE ASSESSMENT

Life-Cycle Assessment (LCA) is a tool for analyzing the environmental burden of products at all stages of their life cycle, "from cradle to grave" – extraction of resources; production of materials, product parts, and the product itself; use of the product; and management after discarding, either by reuse, recycling, or final disposal. Over the last decade, the U.S. and European branches of the Society of Environmental Toxicology and Chemistry[1] (SETAC) have led the intensive development of LCA methodologies, producing a "Code of Practice" – the first internationally accepted technical framework for LCA. This SETAC work is the basis for the LCA protocol in the ISO 14000 environmental management standards of the International

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[1]SETAC, a worldwide professional society, was founded in 1979 to provide a forum for individuals and institutions engaged in the study of environmental problems, the management and regulation of natural resources, education, research, and development, and manufacturing and distribution.

Organization for Standardization (ISO). SETAC defines the inherent features of LCA as follows [1-3]:

- A system-wide or "cradle-to-grave" perspective, implying coverage of the multiple operations and activities throughout a life cycle;
- A multimedia perspective, implying coverage of resource use and emissions to different environmental media (e.g., air, water, and soil); and
- A functional unit accounting system that normalizes energy carriers, material resources, emissions, and wastes across the system (i.e., full fuel cycle) and across media after unit process allocation procedures. Only those percentages of emissions or resource use specific to the function are included in the balance sheet (LCA inventory table).

The methodological framework accepted worldwide for LCA currently recognizes four distinct components of a life-cycle assessment. The first step is a *goal definition and scoping* activity that serves to define the specific objectives and the expected products of a given study, as well as to identify time and spatial boundaries, boundary conditions and assumptions, and impact and improvement objectives. The second step, *inventory analysis*, quantifies and catalogs the materials and energy used and the environmental releases arising from all stages of the life of a product or process, from raw material acquisition to ultimate disposal. The third step, *impact assessment*, examines potential and actual environmental, human health, and resource depletion effects related to the use of resources (energy and materials) and environmental releases. The fourth step (optional) is an *improvement assessment* of the changes needed to bring about environmental, human health, and/or resource management improvements in the product or process. The scope of the current project is limited to the first three steps.

LCA GOAL DEFINITION AND SCOPING

Two major goals are pursued by the current LCA analysis:

- To create an "environmental footprint" of an IGCC-based multi-product system with CO_2 recovery and
- To compare that footprint with that of a conventional IGCC-based system with only electricity generation.

For consistency of analysis, both plants are assumed to be located in Stevens Point, Wisconsin, and fueled by coal from a seam near Sesser, Illinois. To reflect the full life-cycle concept, both analyzed systems include three distinct activity areas, as shown in Figure 2:

1. Production plant (including gasification, gas conversion and purification, and power production by combined cycle);
2. Auxiliary operations and activities (including extraction and processing of coal and other significant major natural resources, transportation of major consumables and construction materials to the power plant, by-products and waste transportation/disposal/reuse, and production of power plant consumables and construction materials); and
3. Power plant construction and demolition, as well as construction of hydrogen and CO_2 transportation pipelines.

DESCRIPTION OF INVENTORY
COLLECTION AND ANALYSIS

To perform the LCA, an inventory of raw materials, products, and emissions associated with activities within this scope was collected for the base and the co-product cases. This inventory has been allocated to the products as described below.

Inventory Collection

Inventory collection and analysis were performed by using the LCAdvantage[TM] computer program developed by Battelle [4]. LCAdvantage[TM] combines life-cycle modeling features with a graphical user interface, database structure, and calculation engine. The LCAdvantage[TM] database comprises materials inventories based on U.S. experience for the production of basic commodities, including power generation, fuels production and distribution, and cradle-to-grave operations for such selected products as metals, cement, and basic chemicals. The quantities of materials, consumables, and effluents associated with IGCC process operations, as well as the pollutant emissions from relevant activities, were obtained from various sources, including the Aspen[TM] simulations, supplemental mass and energy balances, the LCAdvantage database, other reports on LCA analyses, literature, EPA resources, and personal communications with individuals and experts in different industries. The LCAdvantage creates an inventory for all processes involved in construction, operation, and demolition of the plant. The inventory categories are resources, products, and airborne, liquid, and solid residues.

Shell Gasification Combined-Cycle Plant

The major process streams from the Shell gasification combined-cycle plant that need to be considered in the life-cycle assessment are:

- Major resource inputs: coal, water, MDEA and Selexol (used for removal of H_2S and CO_2 from flue gas), catalyst for the reduction of H_2S to elemental sulfur (Claus process), catalyst for chemical reduction of SO_2 to H_2S (SCOT process) to improve total sulfur removal by the Claus plant, and auxiliary electricity.
- Major products: electricity, hydrogen, CO_2, and by-product sulfur.
- Solid waste: coal slag, spent Claus and SCOT catalyst, and dewatered sludge from raw water coagulation process.
- Liquid waste: gasifier blowdown, scrubbing processes blowdown, HRSG blowdown, cooling tower blowdown, and water treatment unit blowdown.
- Airborne residues: SO_2 and CO_2 from SCOT plant stack (base case only), stack gas from combustion turbine, de-aerator vent, N_2 from the air separation unit, and solid particulate drift from the cooling tower.

Auxiliary Operations and Activities

Both cycles include the following processes: coal mining, coal cleaning, coal transportation to the power plant, solid waste collection and transportation, power generation and transmission, and wastewater treatment. In addition, for the multi-product system we include separation of H_2 and CO_2 and delivery of these products to clients via pipelines.

Run-of-mine Illinois #6 coal, mined underground at Sesser County in Illinois, is used in the ASPEN modeling to fuel both plants. Coarse cleaning at the mine mouth is assumed, with refuse returned to the mine. Coal is transported to the plant by rail only. Emissions associated with coal transportation to the power plant include those from diesel fuel use and open rail cars loaded

with crushed coal. We do not include emissions associated with manufacturing of diesel fuel and with manufacturing and maintaining rail cars.

It is assumed that power plant solid waste (slag, solids from water treatment, and spent catalysts) is collected in a dewatering pond located on the plant site. After dewatering, this waste is transported to a landfill 40 to 80 km from the power plant. The landfill is designed to prevent leachate, so emissions from solid waste collection and landfill are only from the fuel used for solid waste transportation by rail. Usually, sulfur produced in the Claus cycle is stored at the power plant and sold to clients. No emissions are expected from the sulfur storage process. Finally, depending on the selected water treatment process, most wastewater does not require treatment before being discharged.

Construction and Demolition of the Power Plant
Hydrogen and CO$_2$ Pipelines
The power plant construction and demolition analysis applies to both power plant cases. The amount of materials required for the construction of a power plant is broadly proportional to the size and complexity of the plant. The bulk construction materials required are steel, cement, and aggregates in the ratio 1:1:6. Other materials include aluminum, copper, glass, and iron, but in insignificant amounts compared to the first three materials. We have assumed that construction of the co-product and base-case plants would require equal amounts of construction materials. The gasifier sections for these plants are identical. Also, the reduction in material use for the power island of the co-product case is offset by the increase in material use for enhanced gas treatment. Fuel use and emissions from the production of these construction materials have been estimated based on the energy required to produce the materials. In addition, we have included fugitive emissions of particulates during construction. Decommissioning will involve some expenditure of energy, depending on the future use of the site. One study advised [5] that the net energy consumption for decommissioning is approximately 10% of the energy consumed in construction. There are two primary solid waste outputs from decommissioning. One of them is scrap metal, which will be partially reused for steel manufacturing. The second is spent shift, SCOT, and Claus catalyst, plus resins from the water treatment unit. This flow of material will be directed to the solid waste module.

Amounts of materials and energy required for power plant construction and demolition activities, as well as emissions associated with these activities, were calculated on the basis of information presented in Gorokhov et al. [6]. All emissions associated with plant construction and demolition were distributed over the assumed 30-yr plant life (alternatively, they could be assigned to the construction period before power plant commissioning and to a demolition period after plant decommissioning).

Construction of H$_2$ and CO$_2$ pipelines is included in the scope of analysis. Both pipelines are assumed to be 100 km long. Initial pressurization of both gases before they are sent from the power plant enables delivery without booster compression. Resources used in the LCA analysis for these pipelines include steel and concrete, as well as energy for manufacture and delivery. Accordingly, emissions associated with construction of pipelines include emissions from manufacturing and delivery of materials. We assume that the pipelines will not be demolished.

Emissions Allocation

A consistent way to compare the environmental performance of alternative plants is to report emissions per unit of production (e.g., per kilowatt-hour (kWh) output for the power generating plant). In the case of multi-product plants, emissions should be somehow allocated to the various products. Then these unit emissions can be compared with those from alternative systems for producing the same products. Unfortunately, there is no standardized or unified system that can be recommended to accomplish this allocation. Our approach is to regard hydrogen and fuel gas as two product fuel streams and allocate emissions according to the energy content of each stream. This allocation is applied to (1) all emissions associated with plant operation before separation of H_2 and CO_2, (2) solid waste collection and transportation, (3) plant construction and demolition, and (4) emissions associated with the construction of the CO_2 transportation line. We view CO_2 as a waste stream, which is to be stored underground. If CO_2 were viewed as a product, the allocation scheme would be more difficult. All emissions associated with operation of the combined cycle are allocated to electricity production (including gas and steam turbines, plant water treatment, and the cooling tower); these include the emissions already allocated to the fuel gas. All emissions associated with construction of the hydrogen transportation line are allocated to the hydrogen flow. This allocation scheme facilitates comparison of the environmental performance of the power production part of the co-product plant with the base-case IGCC plant that only produces electricity. Our previous studies have shown that collection of CO_2 from flue gas and its pressurization for transportation via a pipeline can require a significant amount of additional parasitic power. Thus, *a priori*, both the economic and the environmental performances of a multi-product cycle are expected to be worse than those of the cycle without CO_2 separation. Therefore, an additional comparison of the multi-product IGCC system with an IGCC cycle with separation of CO_2 and electricity-only generation [5] was included in the analysis. These comparisons were made on the per-kWh basis. Environmental performance of the hydrogen-generating part of the multi-product system was compared with the performance of a methane-steam reforming hydrogen-manufacturing process [11] on the per-Btu of generated hydrogen basis.

Emission Inventory Analysis

Bituminous coal and water are the major material inputs. Other fuels and electricity are used mostly for coal extraction and transportation and for solid waste transportation. Although the amounts of steel and concrete needed for plant construction are significant, the per-kWh (per-Btu) amounts, distributed over the 30 years of expected plant life, are several orders of magnitude lower than the amounts of coal and water used for production of electricity.

Emission inventory results for some components are presented in Figure 3. Contributions to emissions by each phase of the process are presented as percentages of the total for each emitted species. On a mass basis, CO_2 is the dominant gaseous emission for the base-case power plant. Most of this CO_2 is produced in the power cycle. In the multi-product plant, more than 90% of the potential CO_2 is captured. Coal extraction and transportation processes result in the next-largest emissions stream, although that stream is two orders of magnitude smaller than the emissions from the power cycle; consequently, total CO_2 emissions from the multi-product cycle are significantly lower. CO_2 emissions are followed in magnitude by CO emissions, also released mainly in the power cycle. Methane released via coal mining represents the third-largest emission. NO_x emissions are associated mostly with coal extraction and

transportation, while SO_x emissions are generated only from the power cycle. Almost all organic emissions identified in the inventory assessment are associated with fuel use for extraction of coal and transportation of coal, waste, and construction materials.

As expected, significant particulate matter emissions are associated with coal extraction and transportation and with the construction/ demolition processes. Note that when the construction and demolition particulates are levelized over the power plant life cycle, the amount (per kWh) is of the same order of magnitude as from extraction and transportation of coal, probably because the construction process includes all emissions associated with extraction of iron ore, development of cement and coke, and transportation of these materials, plus any particulates from the construction site itself. In this analysis, these emissions are distributed over the 30-yr power plant life, while in reality all these emissions are released to the air shed in about a two- to four-year period during power plant construction. Thus, the local impact of these emissions can be very significant. Slag, the most significant solid emission, is expected to have minor impacts, especially since it is a useful by-product.

APPLICATIONS OF LIFE-CYCLE IMPACT ASSESSMENT (LCIA)
IMPACT CATEGORIES

LCIA is a technical, quantitative, and/or qualitative process of characterizing and assessing the environmental effects of plant resource requirements and environmental loadings identified in inventory collection. Strictly speaking, it should address all human health, ecological, and resource depletion impacts. This assessment reports the inventory results as a distillation of inventory loadings and resource use assigned to specific impact categories.

A broad spectrum of impact categories has been developed in the practice of LCIA. The number of selected categories and their nature generally influence the amount of work required to perform the LCIA. On the basis of previous experience [6], 12 categories are selected as the most important for the evaluation of power cycles. These are identified below, aggregated into three broad impact groups:

Natural Environment -   Acidification, eutrophication, smog, global climate changes, and
                          ecotoxicological impacts (aquatic and terrestrial toxicity);
Human Health -   Toxicological impacts, PM_{10} inhalation effects, and carcinogenic
                          impacts; and
Natural Resources-   Depletion of fuels and water.

Some products, resources, or emissions can be involved in more than one impact category. The same emission/product may contribute to two or more exclusive categories in a parallel or sequential manner, and the emission should be divided or allocated to the relevant categories to avoid double counting. It is also possible that the product or result of an effect in one impact category may be the starting point for another effect in another impact category. To deal with such complexities, LCIA procedure in this project was simplified by (1) accounting for primary emission impacts only and (2) not distributing a particular product/emission among a number of different applicable impact categories, but rather assigning the full value of that product/emission to each applicable category, to determine the worst-case impact.

The relative significance of each environmental loading is represented by category indicators, which usually incorporate a spectrum of results ranging from technical values to subjective judgments. These indicators are the basis on which comparisons can be made, so the value of a comparison depends on the varying technical strength and relevance, as well as the degree and type of subjective judgment used to derive a particular indicator. Some indicators can be estimated as a total amount of a single material or emission, such as water use or PM_{10} emission. Other indicators can represent the total amount of different species. For example, land depletion resulting from landfilling of waste can be represented by the total space occupied by all types of landfilled solid waste. In many cases, data on individual chemicals or resources within an impact category must be combined, using so-called "equivalency factors." These equivalency factors express the relative hazard potential of different chemicals within an impact category, but they do not represent actual environmental impact. SETAC and other organizations have developed numerous equivalency factors and provided recommendations for development of new equivalency factors. A brief description is provided below for each impact category, together with the list of inventory items assigned to this category, as well as a basis for calculating category indicators with the relevant equivalency factors.

Acidification
Acidifying substances cause a large diversity of impacts on soil, groundwater, and surface water organisms, ecosystems, and materials (buildings). The most important acidifying compounds are SO_2, NO_x, and NH_3. Acidification potentials (APs) based on H^+ equivalents are used as equivalency factors to calculate the total indicator for acidification. The total indicator score is expressed in kilograms of SO_2 equivalents.

Eutrophication
This category includes all impacts caused by excessively high levels of macronutrients in the environment. Nitrogen (N) and phosphorus (P) are the most important eutrophicating elements. Eutrophication potentials (EPs) are used as equivalency factors to calculate the total indicator for eutrophication. The EPs reflect the potential contribution of a substance to biomass formation and are expressed in kilograms of PO_4^{3-} equivalents. Major contributors to this impact for both power cycles are ammonia and NO_x.

Smog or Photo-Oxidant Formation Impact
Photo-oxidants can be formed in the troposphere via photochemical oxidation of volatile organic compounds (VOCs) or carbon monoxide (CO) in the presence of NO_x and under the influence of UV light. Ozone is considered to be the most important oxidant. The Maximum Incremental Reactivity (MIR) scoring system, developed by W. Carter, is used to calculate the total indicator for the formation of photo-oxidants, converted to kilograms of ozone formed [3].

Global Climate Changes
Global warming is the impact of fossil fuel emissions on heat radiation absorption in the atmosphere. Major contributors are CO_2, methane, and N_2O. Global Warming Potentials (GWPs) are used as equivalency factors, to convert all emissions into kilograms of CO_2-equivalent [3].

Ecotoxicological Impacts

These impacts are the effects of toxic substances on aquatic and terrestrial ecosystems. Only emissions to water and soil are taken into account in this category. Emissions to water are considered to be toxic only for aquatic ecosystems, and emissions to soil are considered to be toxic only for terrestrial ecosystems. Toxicity factors for these toxicity impact criteria were calculated using a combination of the toxicity, persistence, and bioaccumulation properties of the inventoried chemicals to assess their potential fate and environmental effects. Data used for terrestrial toxicity and aquatic toxicity were lowest rodent LD_{50} (mg/kg) and lowest fish LC_{50} (mg/L) [8,9].

Toxicological Impacts on Human Health

This impact category reflects the effects of toxic substances on humans. There are different ways for these substances to enter the human body (inhalation, water, food, etc.), but only the inhalation and water effects are evaluated here. Factors for these toxicity impact criteria were calculated using Toxic Equivalency Potentials (TEPs), which indicate the relative human health risk associated with the release of one pound of a chemical, compared to the risk posed by release of a reference chemical. In this risk scoring system, all releases of carcinogens are converted to pounds of benzene-equivalents; all releases of chemicals that cause non-cancer health effects are converted to pounds of toluene-equivalents [3].

PM_{10} Inhalation Impact

PM_{10} inhalation affects human health via chronic and nonchronic (short-term) respiratory diseases, increasing both human mortality and morbidity rates in exposed areas. The equivalency factor was estimated as the total weight of solid particulate matter released to the atmosphere.

Depletion of Fuel and Water

These categories characterize depletion of so-called abiotic resources. The basis for resource depletion equivalency factors is the inverse of sustainability, which can be expressed as the world annual production of a mineral or a fossil fuel divided by the world reserve base [3,8]. For example, the fossil fuel data, based on global reserves and production, were obtained from Ref. 10. The calculations include all types of fuel used in the power cycle, as well as in all other activities for manufacturing and transportation of all materials included in the inventory.

Depletion of Land

This impact category focuses only on the loss of land as a result of coal mining or other fuel development operations, and on the use of land for landfilling of waste. Because no specific place and type of coal mining were chosen, only use of land for waste landfills was evaluated in this project. The land-use equivalency factors for solid waste disposal are based on the estimated volume calculated using the specific gravity of each type of solid waste. Inventory data for solid waste are expressed in kg/kW (kg/Btu); multiplication of the weight and the inverse of the specific gravity give an indicator of the waste volume per kilowatt, and thus, the landfill volume required per kilowatt of developed energy, or per Btu of generated hydrogen.

LIFE-CYCLE IMPACT ASSESSMENT (LCIA) RESULTS

A comparison of unweighted impact scores for all impact categories is presented in Tables 5 and 6. Table 5 contains data for electric energy generation in three power cycles – base-case IGCC cycle (column 1), multi-product IGCC cycle with separation of CO_2 (Column 2), and an electricity-generating IGCC cycle with CO_2 separation modeled by the IEA [5] (Column 3). Column 2 presents data for the combined-cycle part of the multi-product system. The last two columns in this table represent a shorthand way of comparing the electricity-generating part of the multi-product IGCC cycle with the base-case IGCC cycle and with the IEA IGCC cycle with CO_2 separation in terms of environmental impacts. If values in this column are substantially larger than one, the multi-product cycle has greater environmental impact than the base-case or IEA IGCC cycle. Values within 20% of unity indicate that the impact potentials of the two cycles are not distinguishable [13]. Results in the column Case B/Case A show that the combined cycle of the multi-product system has significantly higher environmental performance than the base case in such categories as eutrophication and toxicity (better reduction of acids and NO_x), GCC (more than 90% of CO_2 captured), and water use (steam-generating cycle significantly smaller than in the base case). On the other hand, its impact in such categories as PM_{10}, smog, air toxicity, land use, and resource depletion is much higher, because overall efficiency of the cycle is less due to the additional auxiliary power required for CO_2 pressurization. Results in the column B/C show that the performance of the multi-product plant for electricity generation is better than that of the IEA-developed IGCC cycle with CO_2 capture in 7 of 13 categories.

Table 6 compares the environmental performance of the hydrogen-generating part of the multi-product system with that of a methane-steam reforming hydrogen-generating process. Results in column 3 show that the multi-product system is superior to the methane-steam reforming process in almost all categories, except for land use and PM_{10} emissions. The higher impact of the multi-product system in the land use category occurs because the methane-steam reforming process generates minimal solid waste. PM_{10} emissions are mostly associated with coal mining and transportation, as well as with construction and demolition of facilities. In addition to the absence of PM_{10} emissions associated with coal processing and transportation, the methane-steam reforming facility is much smaller and accordingly requires fewer raw materials (steel, cement, and aggregates) and activities for construction and demolition. A significant difference in the resource depletion category can be explained by the fact that the indicator for this category is based on a ratio of annual production of fuel to its reserves. This ratio for coal is several orders of magnitude smaller than the ratio for natural gas, the main raw material for the methane-steam reforming process.

Figures 4 and 5 show the comparison of emission impact scores for the different processes in five major emission impact categories.

CONCLUSIONS

- This process design employs a Shell IGCC cycle in a "Vision 21" multi-product plant with low greenhouse impact. Hydrogen can be cogenerated with electricity and delivered to consumers at very high purities. The selection of a very high purity hydrogen product stream benefits the high-efficiency performance of fuel cells while still meeting the internal power needs of the IGCC and having a revenue stream from electricity sales. The introduction of

"shift" to increase the hydrogen content of the gasifier product also benefits the CO_2 recovery, which has inherent cost advantages if it is largely removed prior to the combustion turbines.

- Based on emission inventory analysis, the most CO_2, CO, and SO_2 are generated in the IGCC cycle, methane emissions are mostly associated with coal mining, and particulate matter is mostly generated in construction and demolition of the plant and pipelines. Transportation and mining are responsible for NO_x emissions.

- Environmental performance of the electricity-generating part of the co-product system is similar to that of the IGCC-based cycle with CO_2 removal. However, the co-product plant has larger environmental impact than a base-case IGCC system without CO_2 removal in almost all impact categories, because of the higher auxiliary power requirement connected to CO_2 pressurization before its output from the power plant. Removal of CO_2 and deeper reduction of acid gas emissions makes the multi-product system better in the GCC, toxicity, and eutrophication categories.

ACKNOWLEDGMENT

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Table 1. Comparison of Design Basis for Three Power Cycles

Process	Base Case	Co-Product Case	IEA Case
Gasification	Shell gasification with cold gas cleanup. Raw gas is produced at 1,844°F and 352 psia.		Texaco gasification with cold gas cleanup. Raw gas is produced at 788° F and 711 psia
Ash removal	This is a slagging gasifier with slag quench.		
Air separation	Cryogenic air separation with partial integration (N_2 used as diluent for combustion turbine)		
High-temperature gas cooling/particulate removal	Used to raise high-pressure, superheated steam	Also used for combustion turbine fuel gas preheat	Used to raise high-pressure, superheated steam
COS hydrolysis	Single stage to form H_2S and CO_2		Not applicable
Shift reaction	Not applicable	Two-stage shift to convert raw gas to high H_2 and CO_2 content	Three-stage shift to convert raw gas to high H_2 and CO_2 content
H_2S recovery	MDEA	Glycol used for improved selectivity (H_2S vs. CO_2)	Glycol/ether used
Acid gas treatment	Claus-SCOT using filtered raw gas as SCOT reagent	Claus-SCOT using H_2 product as reagent	Claus plant
CO_2 removal	Not applicable	Glycol	Glycol/ether
H_2 purification	Not applicable	Pressure Swing Adsorption	Not applicable
Combustion turbine fuel	Synthesis gas cleaned of sulfur and particulates	Residual gas rejected by PSA	Synthesis gas cleaned of sulfur and particulates
Steam cycle heat source	Gas turbine exhaust	Gas turbine exhaust and heat recovery from shift reaction	Gas turbine exhaust and heat recovery from shift reaction

Table 2. Comparison of Plant Performance for Three Power Cycles

Item	Base Case	Co-Product Case	IEA Case
Coal consumption, ton/day	3,171	3,171	4,823
Gas turbine power, MW	272.3	62.0	456
Steam cycle power, MW	188.8	91.5	354
Internal power consumption, MW	- 48.3	-77.4	-155
Net electricity, MW	412.8	76.1	646
H_2 production (equivalent MW)	0	423.2 – 100% effic. 275.1 – 65% effic. 194.7 – 46% effic.	0
CO_2 product, ton/day	0	6,612	11,767
CO_2 emissions, ton/day	7,412	800	1,384

Table 3. Coal Mining and Cleaning, Rail Transport and Delivery to IGCC

11-Coal Preparation	As-Received Basis, wt %			Raw Coal	Coal to train	Coal to pulverizer		Coal to gasifier
	Raw Coal wt%	Clean Coal wt%	Dry Coal wt%	ton/d	ton/d	ton/d	ton/d	lbs/hr
Ultimate Analysis				4967	3179.197	3171.00	2977.06	248,088.52
Moisture	10.10	11.12	5.33		353.527	352.62	158.68	13,223.12
Ash	26.19	9.70	10.33		308.382	307.59	307.59	25,632.25
Sulfur	3.68	2.51	2.67		79.798	79.59	79.59	6,632.68
MAF Values								
83.15 Carbon	48.984	63.751	67.904		2026.773	2021.548	2021.548	168,462.29
5.87 Hydrogen	3.458	4.501	4.794		143.081	142.712	142.712	11,892.65
1.63 Nitrogen	0.960	1.250	1.331		39.731	39.629	39.629	3,302.39
0.38 Chlorine	0.224	0.291	0.310		9.262	9.239	9.239	769.88
8.97 Oxygen	5.284	6.877	7.325		218.643	218.079	218.079	18,173.26
100	100.000	100.000	100.000		2437.490	3171.000	2977.062	248,088.52

Table 4.1 IGCC Major Process Streams

21 - Gasification	1	2	3	4	5		6	7	8	
22 - Heat Recovery	Coal feed	Dust from	Nitrogen for	Steam	Oxygen	TOTALin	Slag	Dust	Raw gas	TOTALout
23 - Particulates	to gasifier	recycle	coal transport					to gasifier	product	
Mass Flow lb/hr	(pulverized)	Str #8						Str #2	(dust-free)	
O2	18,173.26	0.00	151.29	0.00	201,606.00	219,930.55	0.00	0.00	2.89E-08	2.89E-08
N2	3,302.39	0.00	18,714.32	0.00	3,863.23	25,879.93	0.00	0.00	25,878.80	25,878.80
AR	0.00	0.00	105.23	0.00	7,737.82	7,843.05	0.00	0.00	7,843.05	7,843.05
H2	11,892.65	0.00	0.00	0.00	0.00	11,892.65	0.00	0.00	12,799.66	12,799.66
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	375,401.00	375,401.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	22,016.03	22,016.03
H2O	13,223.12	0.00	0.00	7,214.38	0.00	20,437.50	0.00	0.00	8,314.22	8,314.22
CH4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	140.52	140.52
H2S	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6,438.24	6,438.24
CL2	769.88	0.00	0.00	0.00	0.00	769.88	0.00	0.00	1.20E-06	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	797.13	797.13
NH3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12.79	12.79
COS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1,061.33	1,061.33
CARBON	168,462.29	60.75	0.00	0.00	0.00	168,523.04	1,154.16	60.75	0.00	1,214.91
SULFUR	6,632.68	0.00	0.00	0.00	0.00	6,632.68	0.00	0.00	0.00	0.00
ASH	25,632.25	1,348.66	0.00	0.00	0.00	26,980.91	25,624.60	1,348.66	0.00	26,973.26
Total Flow lb/hr	248,088.52	1,409.41	18,970.83	7,214.38	213,207.00	**488,890.14**	26,778.77	1,409.41	460,703.00	**488,890.94**
Total Flow cuft/hr			10,148.1	9,289.4	99,340.37				1,915,340.00	
Temperature F	60.0	640.13	104.0	694.0	204.69		2,500.00	640.13	2,500.00	
Pressure psi	14.7	370.00	400.0	500.0	472.00		367.50	370.00	367.50	

Table 4.2 IGCC Major Process Streams (Continued)

24 - COS Hydrolysis

31 - Shift

41 - H2S Glycol

42 - CO2 Glycol

	8	9	10	11	12	13	14	15
	Raw gas to Hydrolysis	Hydrolysis Product	Shift Feed	Shift Product	H2S Glycol Feed	H2S Glycol Product	CO2 Glycol Clean-Gas	CO2 to Sequestration
Mass Flow lb/hr								
O2	2.89E-08	2.89E-08	2.89E-08	2.89E-08	2.89E-08	0	0	
N2	25,878.80	25,878.66	25,878.66	25,878.66	25,878.66	24,298.90	22,540.23	
AR	7,843.05	7,842.30	7,842.30	7,842.30	7,842.30	6,675.96	5,475.72	
H2	12,799.66	12,799.46	12,799.47	39,689.99	39,689.99	39,689.99	39,689.99	
CO	375,401.00	375,399.00	375,399.00	1,806.73	1,806.73	1,657.77	1,493.95	
CO2	22,016.03	22,772.42	22,772.58	609,777.00	609,777.00	240,935.45	58,778.41	550,999
H2O	8,314.22	1,143.78	1,143.76	1,245.04	1,245.04	31.17	14.99	trace
CH4	140.52	140.51	140.51	133.57	133.57	93.28	62.20	
H2S	6,438.24	6,945.58	6,945.58	6,945.57	6,945.57	89.87	0.14	<1% volume
CL2	1.19923E-06	0	0	0	0	0		
HCL	797.13	0.555	0.555	0.555	0.555	0.148	1.70E-02	
NH3	12.79	3.57E-02	3.570E-02	3.570E-02	3.570E-02	0	0	
COS	1,061.33	14.93	14.93	14.93	14.93	1.70E-02	0	
Glycol-C10H22O5	0	0	0	0	0	5.20E-02	1.30E-02	
Total Flow lbmol/hr	22,071.44	21,665.29	21,665.29	35,010.25	35,010.25	26,267.14	22,023.98	
Total Flow lb/hr	460,703.00	452,937.00	452,937.00	693,335.00	693,335.00	313,472.61	128,055.67	
Total Flow cuft/hr	1,915,340.00	395,716.00	468,999.00	471,273.00	393,819.47	322,464.01	268,406.05	
Temperature F	2500	100	457	100	15	35	19	100
Pressure psi	367.5	327.5	459	440	438	434	428	2100

Table 4.3 IGCC Major Process Streams (Continued)

43 - PSA 51 - Power	14 PSA Feed	16 Hydrogen	17 Turbine Feed	18 Air	19 Flue gas to HRSG
Mass Flow lb/hr					
O2	0	0	0	245,550.56	165,696.81
N2	22,540.23	2.25	22,537.95	803,694.99	826,232.57
AR	5,475.72	0.55	5,475.17	14,080.71	19,555.86
H2	39,689.99	29,767.52	9,922.51	0	0
CO	1,493.95	0.15	1,493.80	0	0
CO2	58,778.41	5.88	58,772.48	0	61,290.44
H2O	14.99	1.00E-03	14.99	0	88,827.63
CH4	62.20	6.00E-03	62.198	0	0
H2S	0.14	0	0.144	0	0
CL2	0	0	0	0	0
HCL	1.70E-02	0	1.70E-02	0	1.70E-02
SO2	0	0	0	0	0.256252
NOx	0	0	0		10ppm
Glycol-C10H22O5	1.30E-02	0	0	0	0
Total Flow lbmol/hr	22,023.98	14,766.75	7,257.25	36,716.24	41,485.74
Total Flow lb/hr	128,055.67	29,776.35	98,279.27	1,063,326.26	1,161,603.57
Total Flow cuft/hr	268,406.05	181,150.06	88,002.16		
Temperature F	19	100	100	70	1213
Pressure psi	428	500	500	14.7	14.9

Table 5. Comparison of Impact Scores for Three Power Cycles

Impact Category	Base Case Cycle * (Case A)	Multi-Product Cycle, Combined Part (Case B)	IEA IGCC Cycle with CO_2 Separation (Case C)	Case B/Case A	Case B/ Case C
Acidification	5.03E-04	3.19E-04	3.46E-04	0.63	0.92
Eutrophication	8.72E-01	9.43E-01	1.13E+00	1.08	0.84
Smog	8.52E-05	7.83E-05	1.08E-04	0.92	0.73
GCC	1.56E+00	4.90E-01	2.80E-01	0.31	1.75
Particulate Matter (PM_{10})	3.27E-04	3.31E-04	4.17E-04	1.01	0.79
Terrestrial Toxicity	8.27E-06	6.55E-07	1.07E-06	0.08	0.61
Human Toxicity (air)	1.11E-02	1.08E-02	1.05E-02	0.97	1.02
Human Toxicity (water)	2.16E-08	3.21E-08	4.26E-04	1.49	0.00
Carcinogenicity (air)	2.02E-08	1.69E-08	1.17E-08	0.84	1.45
Land Use	1.09E-01	1.06E-01	8.69E-02	0.97	1.22
Resource Depletion	5.66E-03	5.53E-03	3.64E-03	0.98	1.52
Water Use	1.43E+00	1.84E+00	3.56E+00	1.29	0.52

*A) Base-case IGCC cycle without H_2 and CO_2 separation; net power output – 412.8 MW.

B) Multi-product system, combined cycle only; net power output – 110.3 MW.

C) IEA IGCC cycle with separation of CO_2; net power output – 646 MW.

Table 6. Comparison of Impact Scores for Two Hydrogen Production Cases

Impact Category	Multi-Product Cycle, Hydrogen Part * (Case D)	H$_2$ Plant (Case E)	Case D/Case E
Acidification	5.50E-08	5.31E-07	0.10
Eutrophication	1.05E-05	4.14E-05	0.25
Smog	1.36E-08	4.21E-07	0.03
GCC	1.81E-05	1.15E-04	0.16
Particulate Matter (PM$_{10}$)	5.91E-08	1.33E-08	4.43
Terrestrial Toxicity	1.54E-10	1.41E-09	0.11
Human Toxicity (air)	1.84E-06	1.23E-05	0.15
Human Toxicity (water)	7.14E-15	3.93E-13	0.02
Carcinogenicity (air)	3.35E-12	2.39E-09	0.00
Land Use	1.79E-05	2.35E-06	7.64
Resource Depletion	9.40E-07	3.02E-05	0.03
Water Use	3.11E-04	3.93E-04	0.79

*D) Multi-product system, hydrogen cycle – 1.86E-06 MBtu/hr.
 E) Hydrogen production, natural gas steam reforming – 2.03E-06 MBtu/hr.

Figure 1. Shell-based Gasification Combined Cycle Plant with Hydrogen and Carbon Dioxide
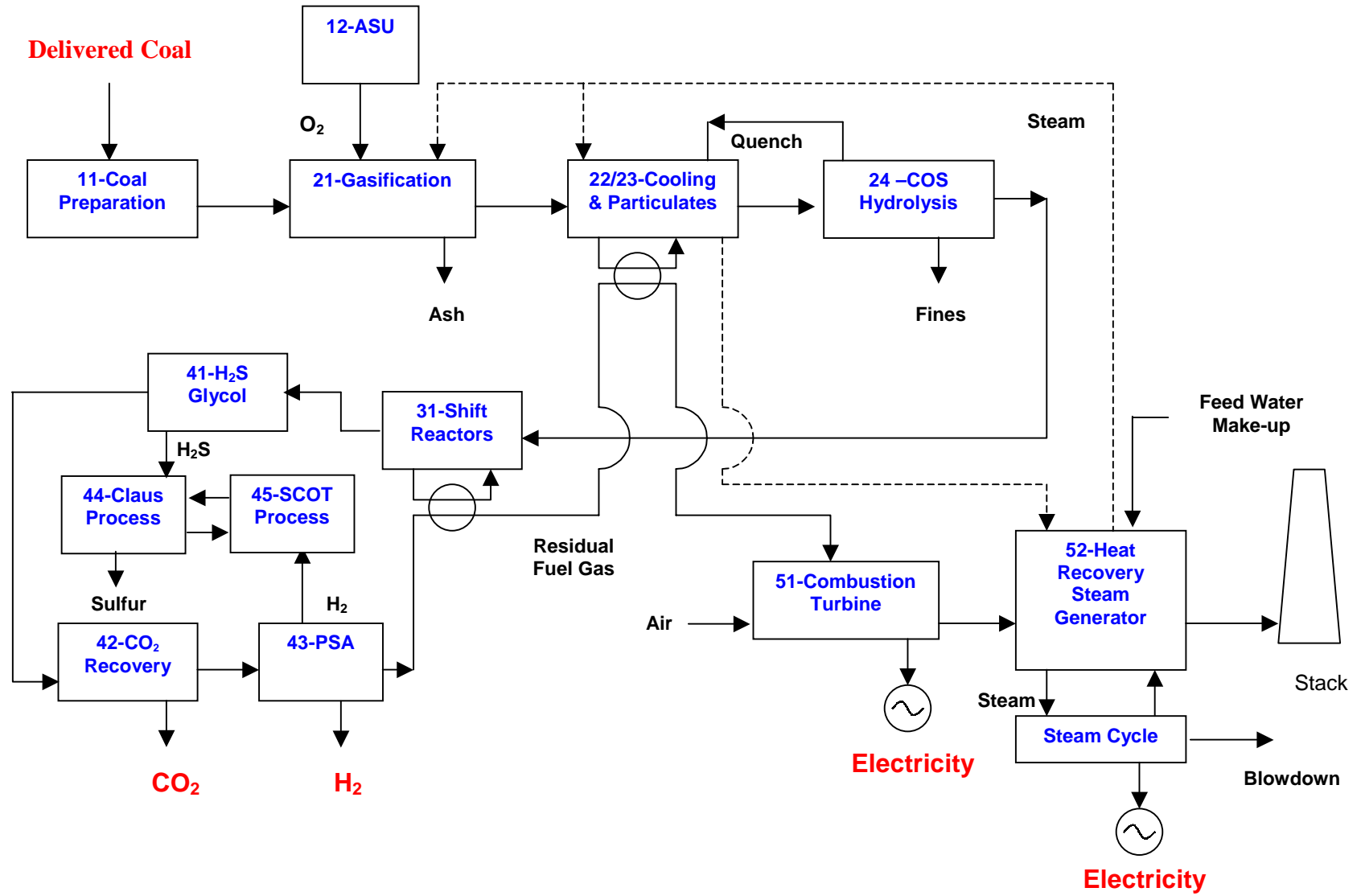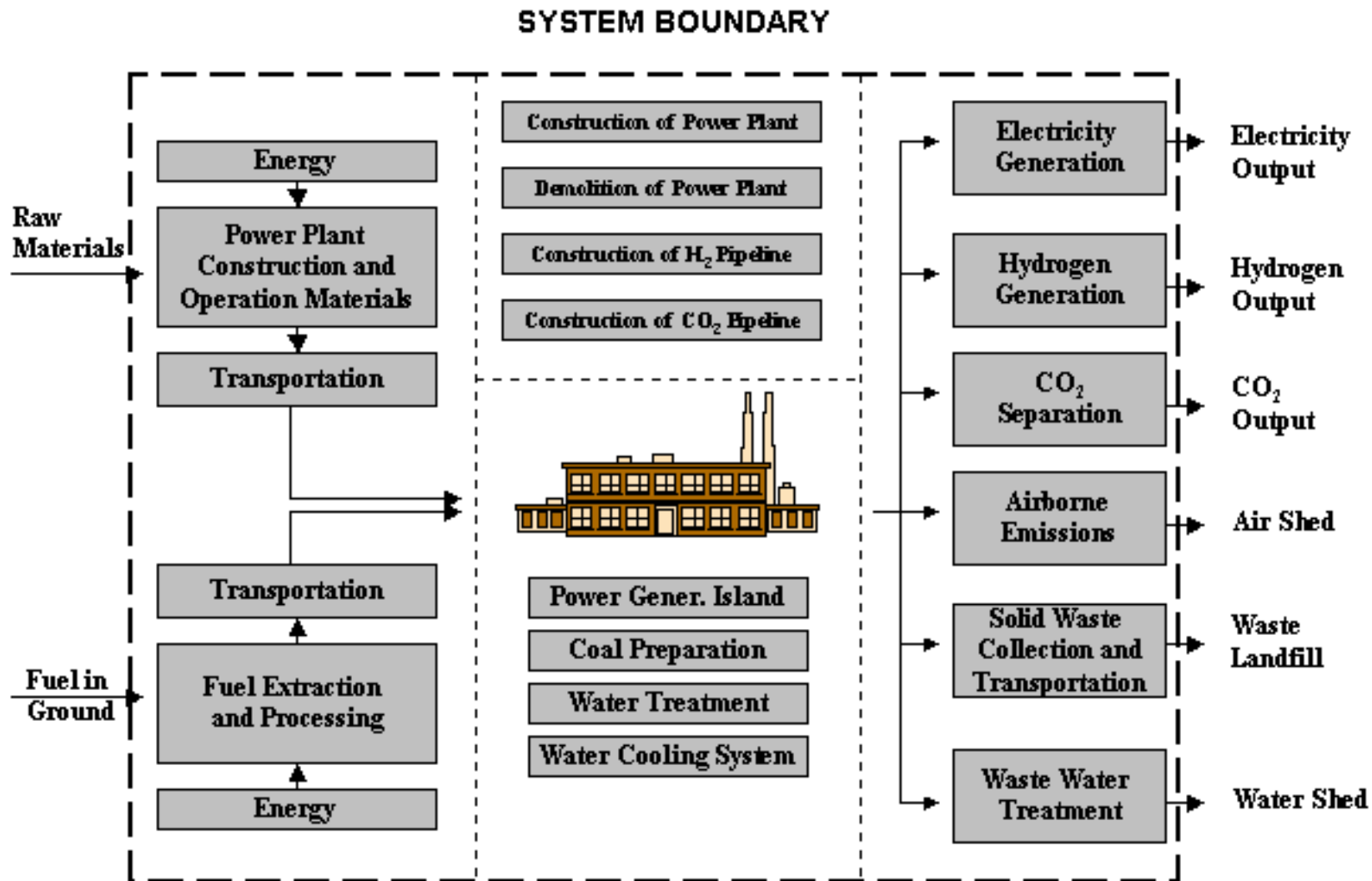
Fig. 2.Coal-fired IGCC-based Multi-product System

SYSTEM BOUNDARY

Raw Materials →

Fuel in Ground →

Energy → Power Plant Construction and Operation Materials → Transportation

Transportation ← Fuel Extraction and Processing ← Energy

Construction of Power Plant

Demolition of Power Plant

Construction of H_2 Pipeline

Construction of CO_2 Pipeline

Power Gener. Island

Coal Preparation

Water Treatment

Water Cooling System

Electricity Generation → Electricity Output

Hydrogen Generation → Hydrogen Output

CO_2 Separation → CO_2 Output

Airborne Emissions → Air Shed

Solid Waste Collection and Transportation → Waste Landfill

Waste Water Treatment → Water Shed

Emission Inventory Analysis
A - Base-case Gasification Power Plant
B - Electricity-generating Part of Multi-Cycle System

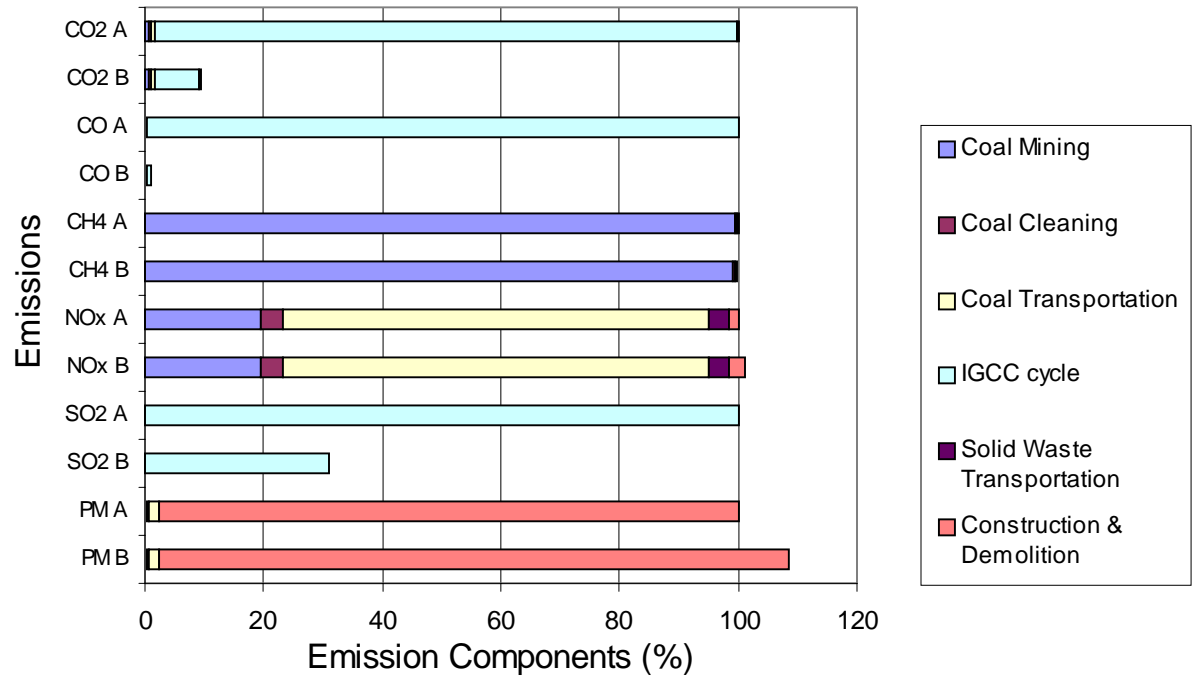**Figure 4. Comparison of Selected Impact Scores for Three Power Cycles**

Relative Impact Values

Case B (Multi-product, electricity)

Case A (Base case)

Case E (IEA)

Smog

GCC

Resource Depletion

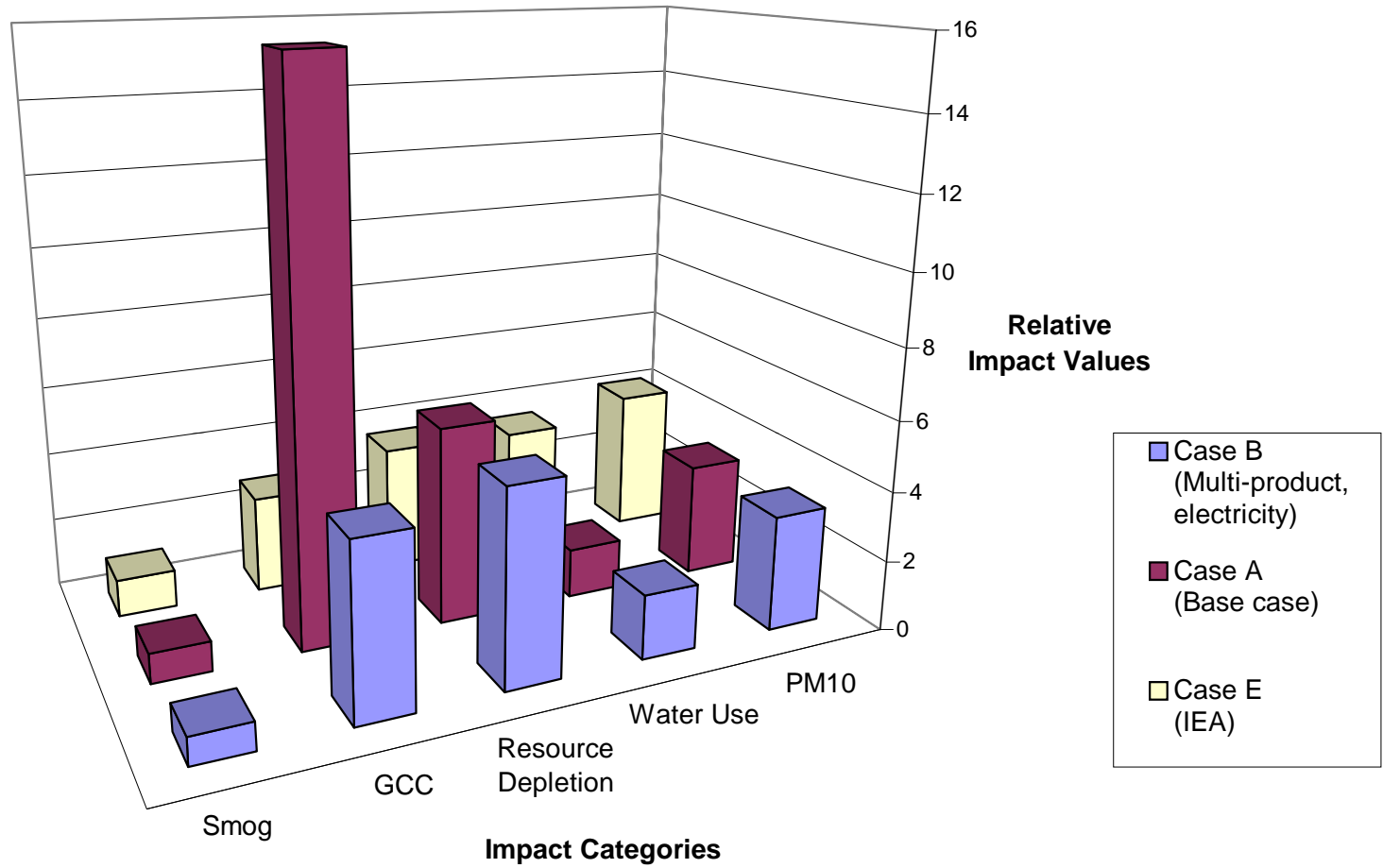Water Use

PM10

Impact Categories

Figure 5. Comparison of Selected Impact Scores for Two Hydrogen Cases