

New Methods for Assessment of Pollution Prevention Technologies: Integration of Probabilistic Process Modeling and Design; Life-Cycle Analysis; and Regional Environmental Benefits Assessment

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Abstract: The objectives of this research are to: (1) develop novel assessment methodologies for evaluation of the risks and potential pay-offs of new technologies that avoid pollutant production; (2) demonstrate the methodology via a detailed case study of one promising new pollution prevention technology; and (3) utilize a tiered approach including process simulation and design optimization, probabilistic analysis, life cycle analysis, and assessment of selected regional environmental impacts to provide insights regarding the risks and pay-offs of the pollution prevention approach, both at a "micro" process-level and at a "macro" regional environmental level. Toward these objectives, activities to date have been to: (1) identify specific process technologies for detailed

evaluation, based upon a solid waste-fueled gasification combined cycle system capable of coproduction of electricity, steam, sulfur, and methanol; (2) develop design bases for major components of the system, including gasification, gas cooling, gas cleanup, gas turbine, and methanol synthesis; (3) implement process simulation models of the major components using ASPEN Plus; (4) obtain and evaluate life cycle inventory data regarding conventional methods for power generation, sulfur production, steam production, and methanol synthesis; (5) develop a corresponding life cycle inventory model; and (6) apply the models to case studies.

Introduction. Technology development is an iterative process involving decisions regarding

which research paths to pursue based upon current results and assessment of competing technologies and market needs. Because of the long lead times (10-20 years is not unusual), decisions on the directions of process development must necessarily be made with incomplete information. Therefore, technology development is inherently a risky enterprise. Risk is the probability of an adverse outcome. Technological risks include high cost, poor performance, and unacceptable impacts to the environment and human health. Due to limited data, there is significant uncertainty during research, development, and demonstration (RD&D) regarding technological risks. Practical formal methods for quantifying and managing these types of technological risks are not available.

With a limited pool of money available to support RD&D, it is urgent that new methods be developed for managing technological development and for evaluating technologies. Now more than ever, we as a society are forced to evaluate carefully how scarce research funds are distributed, trying to invest resources in areas with the greatest possibility of a positive outcome.

The objectives of this research are to:

- (1) Develop novel assessment methodologies for evaluation of the risks and potential pay-offs of new technologies that minimize or avoid pollutant production;
- (2) Demonstrate the methodology via a detailed case study of one promising new pollution prevention technology; and
- (3) Utilize process simulation and design optimization, probabilistic analysis, life-cycle analysis, and integrated assessment of regional environmental impacts to provide insights regarding the risks and pay-offs of

the pollution prevention approach, both at a "micro" process-level and at a "macro" regional environmental level.

The case study is based on a new technology for the production of industrial feedstocks from municipal solid waste (MSW). The technology, waste gasification, has the potential to convey benefits in the areas of avoided chemical production, with additional benefits to electric power generation, production of transportation fuels and avoidance of pollution associated with alternate MSW treatment methodologies. The case study features: (a) efficient resource use through the substitution of solid waste for fossil fuels in the production of a variety of industrial feedstocks and fuels; (b) prevention and reduction of the generation of pollution in the MSW transformation process through better process design, including substitution of gasification for conventional waste-to-energy plants; (c) quantitative approaches to process optimization; (d) reduction of unwanted byproducts associated with both waste management and the avoided industrial feedstock production technologies; (e) development of new process design algorithms; (f) application of probabilistic simulation methods to characterize risks and potential pay-offs of the new approach; (g) quantitative evaluation of the life-cycle impacts of the approach in terms of energy use and air, water, and solid emissions associated with the new waste management alternative; and (h) quantitative evaluation of environmental health impacts, including examples of human health risk reduction.

Motivations and Background: The end products of refining, which serve as feedstocks for the petrochemical industry, transportation sector, and electric power generation, are typically obtained by the use of fossil fuels. These industrial processes have associated environmental impacts throughout the fuel

cycle. New technologies have emerged in the last 10 to 20 years that generalize the notion of refining to a broader array of feedstocks and products. Specifically, gasification technologies offer the flexibility to accommodate a wide range of feedstocks in producing intermediates, including synthesis gas and steam, that can be used in a wide variety of applications. Synthesis gas may be used to generate electricity or to produce a wide range of products such as ammonia, methanol, elemental sulfur, and others. The focus of research in coal gasification has been to decrease pollutant loading and increase thermal efficiency associated with coal utilization. A promising new application of gasification technology involves the substitution of solid waste for fossil fuel feedstocks in making the aforementioned products.

Emerging paradigms for life-cycle analysis (LCA), industrial metabolism, industrial ecology, and sustainable development (e.g., Ayres, 1994; Richards, Allenby, and Frosch, 1994) are placing increased focus on integrated analysis of industrial activities. One application of industrial ecology is to view wastes as raw materials that are significantly underused (Allen and Behmanesh, 1994) and to identify means for making use of the waste for other industrial processes. In MSW gasification, waste utilization will yield pay-offs in terms of avoided (prevented) emissions and discharges from both alternate MSW treatment processes and avoided industrial feedstock production.

The case study also embodies the notion of pollution prevention through better process design. Gasification systems are modular combinations of technologies that serve various functions. The major components typically include feedstock preparation, gasification, heat recovery, gas cleanup, and potentially parallel trains of product and byproduct

recovery steps. Such steps may include gas turbine combined cycle systems for production of electricity and steam, as well as steps for the synthesis of methanol and ammonia, and recovery of materials such as sulfur.

While the primary benefits of waste gasification have been described above, another set of benefits accrues from the substitution of waste gasification for several other common solid waste management options. While it is agreed that a laudible goal is to prevent the generation of MSW through source reduction, it is also recognized that it is highly unlikely that MSW will be eliminated. The most common approaches to MSW management involve landfilling and combustion (EPA, 1996). Combustion is typically associated with waste-to-energy (WTE) plants that produce electricity. WTE plants are relatively few in number compared to the available resource, primarily because of limitations of the underlying technology with respect to cost and public perceptions. In comparison, gasification offers several potential advantages over conventional mass burn waste-to-energy plants including: (1) the prevention of air pollutant emissions, including substantial reductions in dioxins/furans, SO₂, NO_x, HCl, and particulate matter; (2) the potential to "polygenerate" a wide variety of co-products, including electricity, process steam, methanol, ammonia, sulfur, and others, thereby yielding potential economic advantages and avoiding production of these co-products from fossil fuels; (3) substantially higher thermal efficiencies relative to conventional WTE processes; and (4) flexibility regarding the phasing of plant construction and the scheduling of plant operation and co-production operations.

Research Approach

The objectives of this research are to: (1) develop novel assessment methodologies for

evaluation of the risks (cost, technical, environmental, health) and potential pay-offs of new environmental technologies; and (2) to demonstrate the methodology via a detailed case study of one promising new pollution prevention approach.

While there are clearly many benefits of waste gasification from the perspectives of industrial ecology and pollution prevention, there are also risks that must be considered. Because waste gasification is a new concept that has not been fully demonstrated, there are technological risks, including the possibility of poor performance or high cost. In this research, we will develop a procedure to quantitatively evaluate these risks and compare them to the benefits of a successful waste gasification process. Due to the fact that gasification systems involve a combination of highly integrated process areas (e.g., fuel handling, gasification, gas cleanup, combined cycle, byproduct production systems), it is necessary to properly quantify the interactions among such process areas using a process simulation framework. Furthermore, the uncertainties regarding each component, and the variability in feedstock composition and operating conditions, must be considered in developing robust designs.

In this project, we employ methodologies for process simulation and design. Our work includes development of process simulation models for new technologies, including solid waste gasification and unit operations required for "polygeneration" of multiple byproducts.

Life-cycle analysis is used in this work to quantify the energy savings and reduced pollutant emissions associated with waste gasification by the avoided production of the aforementioned co-products from non-renewable resources. A new acid rain integrated assessment model, the Tracking and Analysis Framework (TAF), will be employed

to evaluate the implications of changes in acid deposition precursor emissions that could result from the substitution of waste gasification for conventional waste management, power generation, and chemical production options. TAF includes components for emissions estimation, atmospheric transport and transformations, acid deposition to receptors, estimation of environmental, health, and aesthetic effects, and monetized valuation of the effects. TAF will thus make it possible to use life cycle inventory data for an impact assessment, including lake acidification, incremental changes in human morbidity (e.g., acute human illnesses) and mortality, visibility, and recreational fishing.

The combination of a rigorous plant level process simulation model, life-cycle analysis, and integrated assessment models allows the benefits and risks of a new technology to be evaluated at both "micro" (plant) and "macro" (regional or national) levels. Many life-cycle and integrated assessments make use of simplified assumptions or "coefficients" for a wide variety of model inputs. In this work, such coefficients will be developed based upon the results of a detailed waste gasification probabilistic process simulation and optimization model. This project will emphasize a multi-media approach to minimization of solid waste and air and water discharges.

Overview of Progress to Date

Progress to date on the case study includes several areas. The first is to identify a specific process technology for detailed initial evaluation, which is a solid waste-fueled gasification combined cycle system capable of coproduction of electricity, steam, sulfur, and methanol (Vierrath *et al.*, 1997; Vick, 1996, Philcox and Phenner, 1997; Bjorge, 1997).

A second major area of progress was to develop design bases for major components of the system, including gasification, gas cooling, gas cleanup, gas turbine, steam cycle, and methanol synthesis. The design basis for gasification is based upon moving bed gasifiers that have undergone successful demonstration and operation at the Schwarze Pumpe facility in former East Germany. Both dry ash and slagging fixed bed designs are employed at that facility. Therefore, we have developed design bases for both types of gasifiers. A member of the project team visited Lurgi, the vendor of the gasifier technologies, during a trip to Germany in 1999, in order to obtain the latest publicly available data for use in model development. The gas cooling design basis is predicated upon typical designs employed in integrated gasification combined cycle (IGCC) systems. The gas cleanup system selected as the basis for this study is the Rectisol process, which removes hydrogen sulfide from the syngas produced by the gasifier, and it also removes a significant portion of the carbon dioxide in the syngas. The latter is important to the operability of many methanol synthesis processes. The gas turbine design basis is predicated upon "F" technology gas turbines, such as the Frame 7F design by General Electric. A member of the project team visited General Electric in Schenectady, NY, in November 1998 to obtain the latest available data for development of a model. The methanol synthesis process selected for evaluation in this work is the Liquid Phase Methanol (LPMEOH) process undergoing demonstration at Eastman Tennessee's Kingsport facility. Two members of the project team visiting this facility in September 1999 and obtained the latest available data for use in model development.

A third major area of activity has been the implementation of process simulation models of the major components using ASPEN Plus. Process simulation models have been

implemented and verified for all of the major process areas described above, including: (1) gasification; (2) gas cooling and gas cleanup; (3) gas turbine; (4) steam cycle; and (5) methanol coproduction. The ASPEN Plus models for each process area have been independently verified and calibrated. They also have been combined into a single systems model that allows for integrated assessment of coproduction of electricity and methanol as major products of the gasification of solid waste.

A fourth major area of work has been to obtain and evaluate life cycle inventory data regarding conventional methods for power generation, steam production, and methanol synthesis and to develop the basis for a corresponding life cycle inventory model.

Results to date include development and application of process simulation models of the major components of a waste-based gasification process and associated life cycle inventory models. Where possible, we have obtained real-world industry data through visits to gas turbine and gasification system vendors and through a plant visit to an operating methanol synthesis plant in order to calibrate and/or validate our models. The models now developed enable accurate calculation of mass and energy balances, and environmental discharges, for an advanced technology that offers the potential to substitute solid waste as a feedstock for production of power, steam, and chemicals. The associated life cycle inventory models will enable evaluation of the overall change in life cycle environmental burdens associated with substitution of waste-based gasification for conventional processes. A key benefit of this work is to quantify pollution prevention and life cycle implications when evaluating and designing new technologies.

In the next section we provide some additional details of the results of efforts to date.

Gasification Process Area Model: A gasifier turns a fuel into a synthesis gas ("syngas") that can be used as a cleaner burning fuel or as a feedstock for production of chemicals. Gasification is defined as the thermochemical chemical conversion of a solid carbonaceous feed to a combustible gas product (Chen, 1995). The product syngas is usually rich in hydrogen, carbon monoxide, and various low-weight hydrocarbons. There are three main types of generic gasifiers; fixed (moving) bed, entrained flow and fluidized bed. The differences between classifications are due to movement of the fuel through the vessel, operating pressures and temperatures, size and condition of the entering fuel or a combination of the three. The dry-ash Lurgi gasifier used in this study is a fixed bed type of gasifier. A simple schematic of a fixed-bed gasifier is shown in Figure 1.

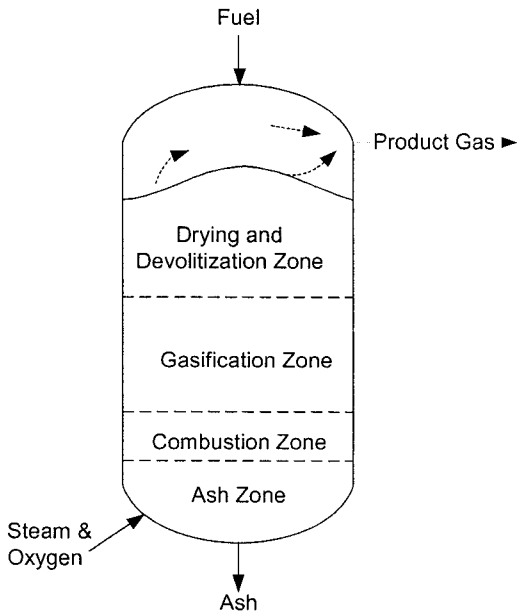


Figure 1. Simple Schematic of a Fixed-Bed Gasifier.

A fixed bed gasifier is currently being used near Berlin, Germany by Lurgi / Shwarze Pumpe, FRG to process solid waste for methanol and power production. The feed is refuse derived fuel (RDF). RDF is made by refining municipal solid waste (MSW) in a series of mechanical sorting and shredding stages to separate the combustible portion of the waste. The MSW is comprised of materials such as plastics, sewage sludge, rubber, fluff, contaminated wood, residues of paint and household waste. The feed does require preprocessing to reduce the size to the required one to three-inch diameter size. The gasification agent is steam and oxygen (Vierrath, 1997).

Based on a previously developed Lurgi dry ash gasifier process simulation model developed by the United States Department of Energy at the Morgantown Energy Technology Center, a gasifier model was developed in ASPEN Plus. The previous model is an air-blown, dry ash fixed bed gasifier incorporated into an integrated gasification combined cycle system with external zinc ferrite desulfurization and selective catalytic reduction. A flowsheet of the newly developed ASPEN Plus model of the gasification process area is shown in Figure 2.

The model represents the gasifier vessel as three major zones, which include devolatilization, partial combustion, and gasification. In the devolatilization zone, lighter hydrocarbons and some fines are removed from the fuel. In the partial combustion zone, a sub-stoichiometric amount of oxygen reacts with the fuel to partially oxidize the fuel. The heat released from the exothermic oxidation reactions is then used in the gasification zone for the primarily endothermic gasification reactions, in which carbon from the fuel, and hydrogen from both the fuel and inlet water or steam, are converted to carbon monoxide and hydrogen. The third major zone shown is a quench vessel, which is

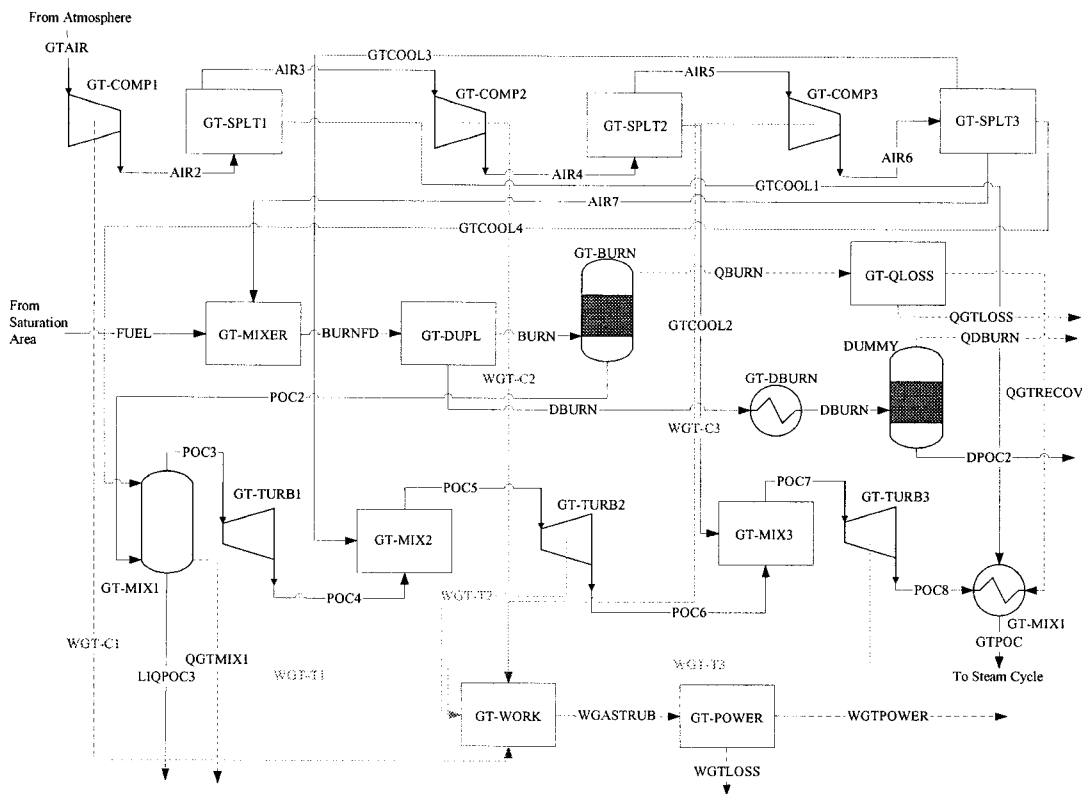


Figure 4. Conceptual Diagram of the ASPEN Plus Process Simulation for the Gas Turbine Process Area.

design basis is representative of Frame "F" gas turbine designs, with firing temperatures of 2,350 degrees Fahrenheit.

Integrated Gasification Combined Cycle System Model. The process areas described here, including gasification, gas cooling and gas cleanup, and gas turbine, are three of the major process area models that have been combined into single process simulation model of a waste-fueled Integrated Gasification Combined Cycle (IGCC) system. The other major process areas for which ASPEN Plus flowsheets have been developed include sulfur recovery, fuel gas saturation, and steam cycle. The development of these process area models is similar in method to that of the ones presented in this paper.

As shown in Figure 5, the IGCC system model includes a fixed bed gasifier, a gas cooling and cleanup system, a gas liquor separator, a Claus

plant and Beavon-Stretford plant for recovery of elemental sulfur, fuel gas saturator, a gas turbine, a steam cycle, and a steam turbine. During gas cooling, some condensates are formed which are separated and treated. Sulfur contained in the fuel is recovered as elemental sulfur. The fuel gas saturator is used to humidify the syngas. Humidification aids in preventing nitrogen oxides emissions from the gas turbine combustor. Also, humidification increases the mass flow rate of the syngas relative to that of compressed air in the gas turbine. The result is that less auxiliary power is consumed by the compressor of the gas turbine compared to the power output of the expander. Therefore, more electricity can be generated from the gas turbine.

The conceptual diagram also illustrates that syngas can be used in a methanol plant to synthesize methanol.

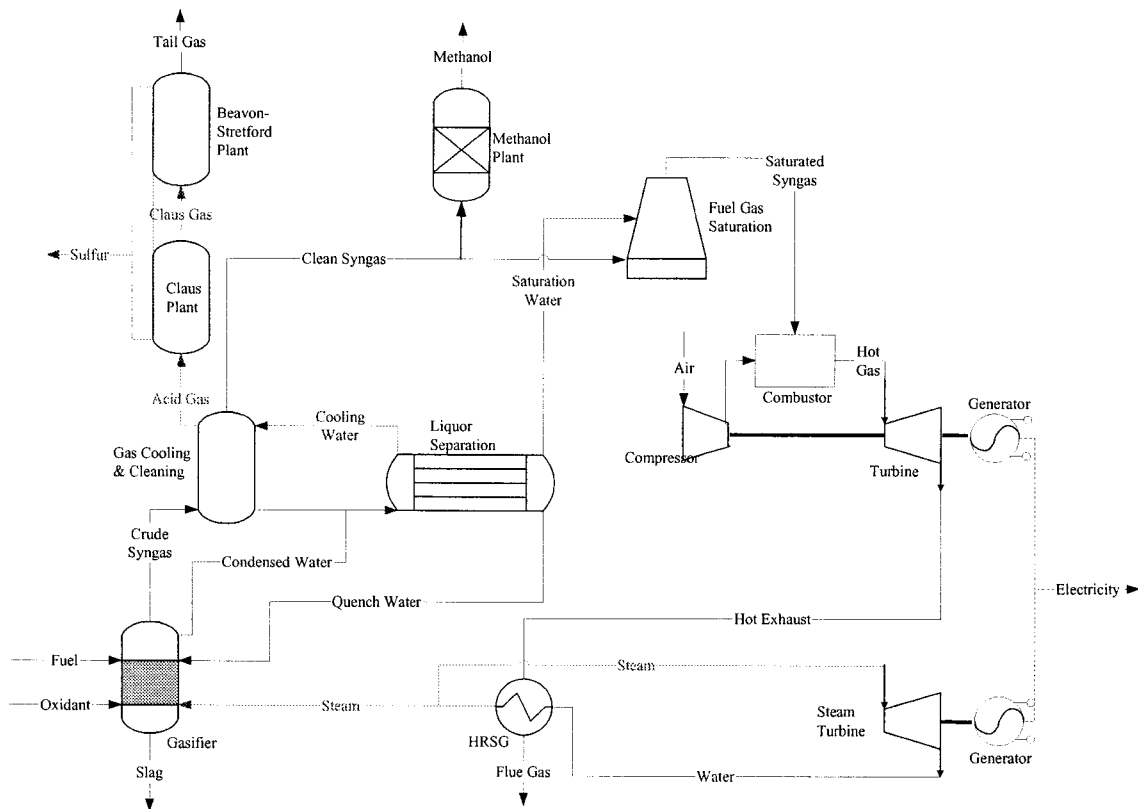


Figure 5. Simplified Schematic of the ASPEN Plus Process Simulation Model for the Waste-Fueled Integrated Gasification Combined Cycle (IGCC) System.

Efforts have been made to verify and calibrate the IGCC system model, based upon published data from a study sponsored by the Electric Power Research Institute for a coal-fueled IGCC system using a similar process design. The results of the verification case study are shown in Table 1.

The results in the table show that the ASPEN Plus IGCC simulation model is able to reproduce the results in the EPRI study, based upon the same input design assumptions, within plus or minus five percent in most cases. The high degree of concordance between the model and the published data is especially significant with respect to overall measures of system performance, such as the total amount of power generated, the plant thermal efficiency, and the mass flows of major streams. While there are some specific areas of

apparent disagreement between the model and the design study, these differences are attributable to differences in the design basis between the two. For example, the simulation model is based upon the use of the Rectisol process for acid gas removal, whereas the EPRI study is based upon a different technology. These differences in design explain the difference in auxiliary power consumption for this particular process area. Overall, the simulation model agrees very well with the published design study.

Methanol Synthesis Process Area Model:

Conventionally, methanol is synthesized in the gas phase reaction over a heterogeneous catalyst from synthesis gas that consists primarily of hydrogen, carbon monoxide and carbon dioxide. Newer processes for methanol

Table 1. Results from the ASPEN Plus Process Simulation Model for a Coal-Fueled IGCC System Compared to Published Results from a Design Study Sponsored by the Electric Power Research Institute (EPRI)

Auxiliary Loads	Power (kW)			To Gasifier	Mass Flow Rates		Percent Error (%)
	ASPEN PLUS	EPRI	Error (%)		ASPEN PLUS	EPRI	
Oxygen Plant	28,717	32,097	-10.53%	Fuel	329,277	318,090	3.52%
Gasification Island	1,067	930	14.73%	Oxygen	182,752	183,012	-0.14%
Liquor Separation	658	650	1.30%	Steam	106,969	106,979	-0.01%
BFW Treatment	615	621	-0.97%	Quench Water	509,961	464,650	9.75%
Fuel Gas Saturation	128	123	4.19%	Crude Syngas	656,304	642,236	2.19%
Beavon-Strefford Tail Gas	446	N/A	-	Clean Syngas to Saturator	516,782	535,483	-3.49%
Acid Gas Removal	7,135	3,180	124.39%	Saturated Syngas	954,101	988,261	-3.46%
Coal Receive & Stor and Prep	1,895	1,792	5.75%	Air to Gas Turbine	6,918,170	6,617,339	4.55%
Liquor Treatment	162	180	-10.14%	Fired Fuel Mixture in Gas Turb.	6,627,100	Not Available	-
Claus Plant	210	w/Acid Gas	-	Overall Consumption of Water	516,777	529,761	-2.45%
Power Island	3,847	3,781	1.73%	Production of Sulfur	10,368	9,892	4.81%
General Facilities*	3,680	3,681	-0.02%	Slag Production	48,274	49,796	-3.06%
TOTAL AUX LOADS (MW)	48.560	48.332	0.47%	Saturation Water	399,578	396,346	0.82%
				Steam for Sat. Heating	301,638	326,634	-7.65%
POWER GENERATION				ENERGY INPUT			
	MW	MW			MMBTU/hr	MMBTU/hr**	
Gas Turbines	384.1	384.0	0.04%	HHV Basis	4,067	3,964	2.59%
Steam Turbines	129.7	135.1	-4.01%	LHV Basis	3,902	3,804	2.59%
Gross Power Generated	513.8	519.1	-1.02%				
Auxiliary Load	48.6	48.3	0.47%				
Power to Grid	465.3	470.8	-1.17%				
OVERALL THERMAL EFF.				HEAT RATE			
					BTU/kWh	BTU/kWh	
HHV BASIS	39.0%	40.5%	-3.61%	HHV	8,740	8,420	3.81%
LHV BASIS	40.7%	42.2%	-3.60%	LHV	8,387	8,080	3.80%

are focused on the use of CO-rich synthesis gas instead of H₂ rich synthesis gas thereby utilizing cheaper synthesis gas for the production of methanol. One of the promising technologies utilizing CO-rich synthesis gas is the Liquid Phase methanol synthesis process (also known as LPMEOH™) that was conceived by Chem Systems, Inc., in 1975.

The LPMEOH™ technology has been developed by Air Products and Chemicals Inc. since the 1980's, extensively proven in a Department of Energy (DOE) – owned process and hydrodynamics development unit in LaPorte, Texas and selected for demonstration under the DOE Clean Coal Technology Program. The process is not yet commercialized. The demonstration plant at Kingsport, TN began operation in April 1997. It has a four year operating program ending in 2001 during which the LPMEOH Process demonstration plant is expected to meet or exceed the design production capacity of 260 TPD of methanol, The plant will simulate operation of an integrated gasification combined cycle (IGCC) system with coproduction of power and methanol. The test plan also seeks to establish commercial

acceptance of the technology and verify the fitness of the as-produced methanol product (about 98-wt% purity) through a series of off-site, product -use tests.

The production of methanol by a liquid phase process involves three phases: namely, solid phase – the catalyst; liquid phase – inert hydrocarbon or oil; and gas phase – synthesis gas. The reaction takes place in a three phase fluidized bed reactor within the synthesis section of the methanol plant. The catalyst in the reactor is fluidized by inert hydrocarbons. Synthesis gas containing CO, H₂, and CO₂ is passed upward into the reactor concurrent with the inert hydrocarbon. At the top of the reactor, the solid, liquid and vapor phases separate. The catalyst remains in the reactor while the hydrocarbon liquid is separated from both catalyst and vapor and is recirculated to the reactor via a heat exchanger where the cooling occurs by generating high-pressure steam. The effluent gases from the reactor are then cooled and condensed. Hydrocarbon liquid is immiscible with methanol and so is phase separated. The methanol produced can be purified by distillation to produce chemical

Table 2. Life Cycle Inventory of Steam Production, including Pre-Combustion Emissions, Combustion Emissions, Emissions Associated with Lime Use in Spray Dryers for SO₂ Control, and Emissions Associated with Boiler Feed Water Treatment, in Units of kg pollutant/MJ of Steam

Air Emissions	Pre-Combustion Emissions	Boiler Emissions	Lime LCI	BFW LCI	Total (kg/MJ Steam)
PM	2.48E-05	3.03E-06	1.39E-06	6.96E-08	2.93E-05
PM-10	no data	no data	no data	no data	
SO ₂	4.87E-04	6.23E-05	1.90E-06	2.39E-07	5.51E-04
SO ₃	no data	no data	no data	no data	
NO _x	4.11E-05	6.44E-05	6.68E-07	3.26E-07	1.07E-04
CO	6.28E-05	6.41E-05	1.80E-07	1.96E-08	1.27E-04
CO ₂ (fossil)	7.61E-03	8.21E-02	6.68E-04	3.80E-05	9.04E-02
CO ₂ (Biomass)	1.75E-05	no data	2.47E-08	no data	
CH ₄	1.32E-04	3.88E-06	4.88E-07	8.04E-08	1.36E-04
HCl	6.64E-08	no data	6.17E-13	2.17E-09	
VOCs	no data	no data	no data	3.54E-07	
NH ₃	5.89E-08	no data	1.03E-10	no data	
Hydrocarbons	1.92E-04	no data	1.54E-07	no data	
METALS					
Antimony (Sb)	no data		3.75E-13	no data	
Arsenic (As)	no data	1.75E-09	7.71E-11	no data	
Beryllium (Be)	no data	9.00E-11	no data	no data	
Cadmium (Cd)	no data	2.24E-10	2.57E-11	no data	
Chromium (Cr)	no data	1.11E-09	1.59E-10	no data	
Cobalt (Co)	no data	no data	no data	no data	
Copper (Cu)	no data	no data	no data	no data	
Lead (Pb)	2.82E-10	1.80E-09	9.77E-12	no data	
Mercury (Hg)	no data	3.54E-10	2.21E-12	no data	
Nickel (Ni)	no data	2.13E-09	1.08E-10	no data	
Selenium (Se)	no data	5.51E-09	4.11E-13	no data	
Zinc (Zn)	no data		no data	no data	
Liquid Emission					
Dissolved Solids	7.42E-04	0.00E+00	5.66E-07	no data	
Suspended Solids	1.43E-05	0.00E+00	2.21E-08	2.80E-07	1.46E-05
BOD	7.97E-07	0.00E+00	6.17E-10	2.17E-10	7.98E-07
COD	5.56E-06	0.00E+00	8.23E-09	3.04E-09	5.57E-06
Oil	1.35E-05	0.00E+00	9.77E-09	no data	
Sulfuric Acid	1.66E-08	0.00E+00	2.01E-09	no data	
Iron	1.06E-06	0.00E+00	1.08E-08	no data	
Ammonia	2.06E-08	0.00E+00	3.03E-11	no data	
Copper	0.00E+00	0.00E+00	no data	no data	
Cadmium	3.37E-08	0.00E+00	2.67E-11	no data	
Mercury	2.65E-12	0.00E+00	2.06E-15	no data	
Phosphate	8.42E-09	0.00E+00	9.77E-10	no data	
Selenium		0.00E+00	no data	no data	
Chromium	3.37E-08	0.00E+00	2.57E-11	no data	
Lead	2.10E-11	0.00E+00	7.71E-15	no data	
Zinc	1.19E-08	0.00E+00	8.74E-12	no data	
Solid Waste	4.43E-03	1.02E-03	1.57E-03	1.93E-03	8.95E-03
Energy (MJ)	1.36E-01	1.23E+00	2.76E-03	6.59E-04	1.37E+00

The LCI models for methanol production take into consideration the mass and energy balances of methanol production. Emissions associated with purge gas streams are considered. Fugitive emissions are estimated. LCIs for steam and electricity are included.

Current and Near-Term Future Work: At this time, the IGCC and LPMEOH ASPEN Plus simulation models have been integrated. Work is underway to complete sensitivity analysis case studies of the gasification co-production system for production of electricity, methanol, and sulfur.

Work is underway to develop process simulation and life cycle inventory models for the production of ammonia. Furthermore, work is underway to complete a life cycle inventory comparison of methanol production from waste-fuel derived syngas versus conventional methanol production from natural gas.

Efforts are underway to include quantitative uncertainty analysis as part of the ASPEN Plus simulation framework. A probabilistic modeling capability for ASPEN Plus has been obtained from Carnegie Mellon University, courtesy of Dr. Urmila Diwekar. This capability is being evaluated for use in case studies aimed at characterizing the technological risk of co-production from solid waste.

Status of the Project: With respect to our proposal, work to date has primarily addressed Tasks 1, 2, 4, and 5. Task 1 focuses on data collection, which has been a major thrust area. As previously noted, we have been proactive in seeking data from industry and have made several trips to facilitate this type of information gathering. We have also collected recent information via conferences and technical reports. Task 2 focuses on process modeling development. Our main activity in

this regard has been process performance and emissions modeling. Task 4 includes model verification and validation efforts, which we have performed and are continuing to conduct. Task 5 involves development and application of life cycle inventory models. During the coming year, we will be making progress also on Task 3, which involves application of quantitative uncertainty analysis to characterize technological risk.

Conclusions: At this time, we have been successful in collecting sufficient data necessary to the development of key process area models of a waste gasification system. We have made decisions regarding which technologies to evaluate for gasification, gas cleanup, gas turbine, and methanol synthesis. We have developed and implemented process area models in ASPEN PLUS, and have completed an integrated model of gasification with co-production of electricity, methanol, and sulfur. Simultaneously, we have collected, evaluated, and analyzed life cycle inventory data, and developed selected LCI models. These models have been verified and applied to base case and sensitivity analysis case studies.

The model development, verification, and sensitivity analysis activities are an essential foundation for continuing work on this project, in which we plan to add to ammonia production to the existing ASPEN Plus simulation model for polygeneration of electricity, methanol, and sulfur. The attendant life cycle inventory models for evaluation of overall shifts in environmental burdens associated with substitution of waste gasification for current conventional approaches to production of these commodities will also be further developed. Quantification of technological risk, and opportunities for optimization of these complex technologies, will be part of the remaining work on this project.

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