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Additional Tests to Upgrade and Refine the Aspen Model for Leaching

2013 TECHNICAL REPORT

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3002000464
Final Report, April 2013

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Acknowledgments

The following organization, under contract to the Electric Power Research Institute (EPRI), prepared this report:

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This report describes research sponsored by EPRI.

Most of the research and technical work described in this report was performed by Dr. Stylianos Arvelakis of Thermorefinery Technologies LLC, a contractor of EcoLogix Group. EPRI gratefully acknowledges the contributions of EcoLogix and Thermorefinery Technologies.

This publication is a corporate document that should be cited in the literature in the following manner:

Additional Tests to Upgrade and Refine the Aspen Model for Leaching. EPRI, Palo Alto, CA: 2013. 3002000464.

Abstract

Leaching of biomass to reduce or eliminate troublesome constituents—such as alkali metals, chlorine, sulfur, and phosphorus—presents the opportunity to solve many of the problems involved in the firing, co-firing, or gasification of low-cost, low-grade agricultural biomass and waste materials for energy and biofuel production. The Electric Power Research Institute (EPRI) is interested in fostering the development of this potentially game-changing technology.

EPRI sponsored several laboratory-scale projects to evaluate the leaching process developed by Thermorefinery Technologies. An Aspen Plus[1] model was developed to describe the leaching process and to use with a torrefaction model developed by EPRI. The torrefaction model will be used to develop another model that will describe the integrated torrefaction and leaching process.

Based on the positive outcomes of the initial work, the target of this EPRI-sponsored project is to move ahead by upgrading the leaching process model to be able to better handle all of the different biomass and waste materials available as feedstock in leaching pretreatment. Another objective is to enhance the leaching process model's ability to reproduce experimental results. Accurate reproduction of results will enhance the validity of the model and minimize the need for extensive laboratory testing every time a new biomass or waste material must be integrated into the leaching process model.

As a first step, a small research project was executed to generate more leaching data from three biomass materials from agricultural residues—corn stover, barley straw, and miscanthus. The new data were used to update the model and develop coefficients that can be used to predict the leaching behavior of other biomass materials. This report summarizes the testing, the upgrade to the Aspen model coefficients, and the improvement achieved in predicting the leaching behavior of different biomass materials compared with experimental results.

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[1] Aspen Plus is a registered trademark of Aspen Technology, Inc.

Keywords

Alkali metals
Ash
Aspen Plus model
Chlorine
Leaching
Phosphorus

Executive Summary

Leaching of biomass to reduce or eliminate troublesome constituents—such as alkali metals, chlorine, sulfur, and phosphorus—presents the opportunity to solve many of the problems involved in the firing, co-firing, or gasification of low-cost, low-grade agricultural biomass and waste materials for energy and biofuel production. The Electric Power Research Institute (EPRI) is interested in fostering the development of this potentially game-changing technology.

As part of this endeavor, EPRI sponsored, through its Program on Technology Innovation, a series of small laboratory-scale projects in order to evaluate the leaching process developed by Thermorefinery Technologies (see EPRI reports 1024662, 1022720, and 1024893). Other objectives were to test and select candidates for several parts of the process, such as leaching, mechanical dewatering, drying, and water-cleaning equipment and procedures. These equipment pieces and procedures might be applied in the future in a continuous pilot-scale leaching/washing plant. As part of these research projects, an Aspen Plus[2] model was developed to describe the leaching process and to be used in connection with a torrefaction model developed by EPRI. The Aspen Plus model will be used to develop another model that will describe the integrated torrefaction and leaching process.

Based on the positive outcomes from the initial work performed on the integration of the leaching process, a target of this EPRI-sponsored project is to move a step ahead and upgrade the leaching process model to be able to better handle all of the different biomass and waste materials available as feedstock in leaching pretreatment. Another goal is to enhance the model's ability to reproduce more accurately the experimental results, thereby increasing the validity of the model and minimizing the need for extensive laboratory testing every time a new biomass or waste material has to be integrated into the leaching process model.

As a first step, we undertook a small research project to generate more leaching data from additional agricultural residues' biomass materials. These data were used to upgrade the Aspen Plus leaching

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process model and develop coefficients that can be used to predict the leaching behavior of additional biomass materials. For these data-generating leaching tests, we used three different biomass materials—corn stover, barley straw, and miscanthus from Greece—with deionized water and two different solvents.

The results from the application of the additional experimental data in the leaching model showed that the model's predictions improved. The coefficients used to describe the behavior of the different biomass materials now take better values and fall within narrower limits compared to what we had before.

Unit Conversions

SI Unit	English Unit	Conversion Rate
Pascal	Bar	1 bar = 100 KPa
Degree Celsius	Degree Fahrenheit	°C = (°F-32) x 5/9
Kilogram	Pound	1 lb = 0.45 kg
Liter	Gallon	1 l = 0.264 gal
Millimeter	Inch	1 in. = 25.4 mm
Micron	Mil	1 μm = 0.039 mil
Megajoule/kilogram	British thermal unit/pound	1 BTU/lb = 431 MJ/kg

Acronyms

COD	chemical oxygen demand
DDGS	dried distilled grains with solubles
EPRI	Electric Power Research Institute
HHV	high heating value
ICP	inductively coupled plasma
ISO	International Organization for Standardization
MSW	municipal solid waste
RDF	refuse-derived fuel
SRF	solid recovered fuel

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Section 1: Introduction

1.1 Overview

In the search for alternatives to fossil fuels, biomass is one of the most attractive options. Utilization of biomass as fuel for power production offers the advantages of being renewable and almost CO_2-neutral. Biomass fuels include wood, agricultural residues, and fast-growing trees and crops that can be burned directly in a combustor or can first be upgraded through gasification into a gaseous fuel and then used to produce heat and power. Because agriculture dominates the landscape in most parts of the world, agricultural residues (called *agroresidues*), such as those from straw, olives, hulls, and pods, are the most abundant biomass resource used for decentralized heat and power production. This is especially true in underdeveloped and environmentally sensitive areas.

Agroresidues have the advantage of being truly renewable because they are produced every year. Also, with the exception of straw and grass residues, their production and transportation are inexpensive because they are the natural byproducts of agro-industrial processes. This combination of renewability and affordability makes agroresidues attractive as a source of decentralized energy production.

However, utilization of agroresidues in existing power generation systems and gasification plants is hampered by the potential for undesirable inorganic components in biomass to react unfavorably in existing systems and the difficulty in handling biomass and feeding it into the systems. Applying biomass pre-treatments, such as leaching to eliminate alkali metals and chlorine and to substantially reduce sulfur and phosphorus, will facilitate an increase in the use of agri-waste and other low-cost biomass in co-firing with coal or in 100% biomass-dedicated plants. Further, pre-treatment is expected to avoid fouling agglomeration, reduce the frequency of corrosion problems, and improve efficiency.

1.2 Ash-Related Problems of Biomass

In order for agroresidues to replace conventional fossil fuels, several important operational and environmental aspects must first be examined. The ash behavior of agroresidues during thermochemical conversion is one of the most important matters to be addressed [1, 2]. *Ash* refers to all biomass inorganic constituents in a variety of forms, such as organically bound cations, inorganic salts and minerals, and any other minerals externally bound to biomass feedstocks. Agroresidues contain mainly alkali metals, such as potassium, that may be present as inorganic salts, metals connected to carboxylic or other functional groups, or complex ions or chemisorbed material. As their principal ash-forming, inorganic constituents, silicon—in the form of hydrated silica or deposits on the cell walls—is another common constituent of agroresidues. They are also rich in elements, such as chlorine and sulfur, compared to wood fuels. They contain small amounts of alkali earth materials, such as calcium present in cell walls or occurring as crystalline calcium oxalate in cytoplasm, magnesium, and phosphorous, with the last two present mainly in biological forms [2, 3].

The presence of large amounts of these inorganic constituents in some biofuels is associated with problems such as deposition, sintering, agglomeration, fouling, corrosion, and erosion during the operation of combustion and gasification plants. In particular, alkali metals— especially potassium, which has high mobility—tend to react with silica, even at temperatures far below 900°C by breaking the Si-O-Si bond and forming low-melting-point silicates. Alkali metals also react with sulfur to produce alkali sulfates. Chlorine acts as a facilitator of these reactions, increasing the mobility of potassium, because most of it is present as KCl. Potassium chloride is among the most stable high-temperature, gas-phase, alkali-containing species, whereas the amount of chlorine in the fuel often dictates the amount of alkali that can be vaporized during combustion or gasification. It also appears that calcium reacts with sulfur to form sulfates, but the lower mobility of calcium in combination with its limited quantity in these biofuels does not make it a significant problem [1, 2, 4–6]. The produced alkali silicates and/or sulfates have very low melting points that can reach 700°C and tend to deposit on the reactor walls or heat exchange surfaces in the case of conventional, grate-fired systems. However, in the case of fluidized bed reactors, they contribute significantly to bed sintering and defluidization of the bed inert material through the development of a sticky deposit on the surface of the bed particles [3, 7–9].

Ash-related problems in the form of fouling, slagging, corrosion, and erosion are some of the biggest obstacles to safe, economic, and environmentally friendly utilization of a large variety of biomass and waste fuels (such as straws, hulls, municipal solid waste [MSW], and sewage sludge) for energy generation through thermochemical conversion methods. Furthermore, in the case of MSW incineration plants, the deposition and corrosion processes can also be affected by the presence of heavy metals, such as zinc and lead in the forms of chlorides and sulfates. These compounds have very low melting points—for example, 290°C for $ZnCl_2$, 501°C for $PbCl_2$, and 680°C for $ZnSO_4$—and they interact with compounds such as the KCl and alkali metal sulfates present in large amounts in the ash material produced during MSW incineration. This leads to the formation of molten phases with even lower melting points compared to the pure salts, that is, 250°C for the $ZnCl_2$/KCl (48/52%wt.) mixture, accelerating significantly the deposition and corrosion processes [10–15]. Apart from their contribution to ash-related problems, large amounts of heavy metals (Zn, Pb, Cu, and so on), alkali chlorides, and sulfates in the ash formed during MSW incineration constitute a significant problem in terms of the treatment and disposal of the generated ash material in an economical and environmentally friendly way [16–19].

As a result, it is imperative that the industry develop technologies that will minimize ash-related problems created by biomass and waste inorganic content during thermochemical conversions of these materials for production of energy and fuels. In today's markets, the demand for greater utilization of low-cost biomass and waste materials to mitigate increasing environmental problems, such as the greenhouse effect, is growing fast.

1.3 Leaching History and Literature Survey

Leaching biomass through solid-liquid extraction with water as the extraction method has been shown to improve biomass fuel properties for high-temperature processes and might be a useful process for pretreatment of food processing residues. Water leaching effectively removes water-soluble alkali metals, chlorine, phosphorus, and sulfur from biomass, and it upgrades crude biomass to better-quality feedstock for biofuel and bioenergy production [20, 21]. Leaching biomass with water has been demonstrated to reduce deposit formation during thermal conversion [21–28]. Leaching generally improves the properties of biomass by lowering the ash concentration, increasing the heating value, and altering slag-forming ash compositions [29]. Removing chlorine from biomass reduces acid gas formation, corrosion, and production of toxic species, such as dioxins and furans, during thermal processing [30–32]. In general, large fractions of potassium, sodium, chlorine, sulfur, and phosphorous in biomass fuels can be removed by leaching with water.

Several biomass leaching techniques, such as repeated soaking and draining, have been studied [33, 34]. Another method is to rinse biomass with water, drain it, and mechanically dewater the wet biomass [27]. Biomass leaching can also be done naturally by rain-washing in the field [21–35]. As has been shown, leaching can be performed using any kind of water [34]. Combustion and gasification tests with the water-leached biomass have proven that these materials expand the operation of the reactors by more than 10 times compared to the original untreated biomass materials. Depending on the leaching method and the structure of the biomass, significant amounts of alkali metals, chlorine, sulfur, and phosphorous can be removed within a few minutes, although the fraction removed depends on ion type [20]. Water leaching also removes organic compounds, such as organic acids, water-soluble carbohydrates, and ethanol, from biomass [22].

The possibility of using water-leached biomass in some combustion and gasification applications, such as atmospheric fluidized bed systems, has been successfully demonstrated. However, the limitations of water-only leaching and its limited success in combustion and gasification applications, where higher temperatures and pressures are used, in combination with the higher cost of the leached biomass and the low prices of electricity prevented the commercial application of such solutions until today [22, 26–28].

1.4 Thermorefinery Leaching Technology

Thermorefinery Technologies LLC developed an innovative leaching technology to pretreat secondary biomass (including wheat straw, corn stover, olive residues, rice straw, dried distilled grains with solubles [DDGS], and switchgrass), MSW (particularly refuse-derived fuel [RDF] and solid recovered fuel [SRF][3]), and municipal and industrial sludges so that they can be used in combustion and gasification/pyrolysis systems in the following ways:

- Without ash-related problems
- Without emissions of dioxins and furans
- With significantly reduced emissions of sulfur, NO_x, and heavy metals
- With nutrient (K, P, Cl, and S) recycling back to the ground
- With production of industrial chemicals with substantial economic value that can help to reduce significantly the process cost

The process can produce a clean biomass stream from renewable biomass. This leaching process can also be applied in combination with a torrefaction stage to produce an advanced, clean solid biofuel with superior properties compared to other bio-coal/syn-coal materials as well as the low-grade biomass and waste materials.

The processed clean biomass, bio-coal, and syn-coal have virtually no alkali metals nor chlorine and contain only low amounts of sulfur, phosphorus, and heavy metals compared to the original feedstocks. They have net calorific values of 17–22 MJ/kg in the case of the clean biomass and 20–30 MJ/kg in the case of the clean bio-coal/syn-coal materials' dry basis. These clean biomasses as well as bio-coals and syn-coals can be safely combusted as-is in standard power plants, without the problems typically associated with the original feedstock. Thermorefinery Technologies has applied for four patents for its proprietary torrefaction and leaching processes.

The processes are based on advanced principles of chemistry and thermal processes for the pretreatment of high-alkali, high-chlorine, and sulfur materials to eliminate chlorine and alkali metals and to substantially reduce sulfur, phosphorus, nitrogen, and heavy metals, producing a clean, coal-like, high-calorific-value fuel and/or a clean biomass material.

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[3] The biomass portion of RDF/SRF, typically more than 50%, has monetary value under multiple greenhouse gas protocols, such as the European Union Emissions Trading Scheme.

The full, integrated solution involves the following four-step process:

1. Leaching out troublesome compounds (alkali metals, chlorine, sulfur, heavy metals) from the feedstock
2. Pre-drying the cleaned feedstock
3. Thermal treatment (torrefaction) of the feedstock to induce coalification, increase energy density, and improve grinding properties
4. Densification through pelletizing/briquetting

The leaching step in this project can also be applied after or without the torrefaction-densification treatments based on the specific conditions, such as when the clean feedstock is not to be used in pulverized-fuel boilers for power production or when no long-distance shipping is required. The thermal treatment can actually cause problems if the material has to be fed in fluidized bed boilers as well as in stoker systems where the increased friability of the torrefied material is a disadvantage due to the formation of excessive dust loads if it is not densified.

The leaching process will integrate and use off-the-shelf technology for milling and shredding, leaching baths, leachate liquids processing, and waste treatment.

After pretreatment, the feedstock—its exact attributes depend on the feedstock's original chemical composition—can be directly used for combustion/gasification alone or in combination with coal in ratios of up to 50% and above, to generate electricity and heat, or to produce liquid fuels and chemicals through the Fischer-Tropsch process. The clean feedstock can also be used in other industrial applications, such as metal ore reduction and production of heat and power to meet process needs in various industries.

The leachate will contain chemicals from the biomass (K, Cl, P, S) that can be used as fertilizers. The leachate will also contain chemicals with significant industrial value and provide an extra source of revenue that can reduce substantially the operational costs of the pretreatment.

1.5 Targets for Energy Conversion Applications

Using thermochemical conversion processes, we can now use low-quality biomass and waste materials in a variety of applications for energy and fuel production. These processes include biomass and waste combustion and gasification in fluidized bed boilers and gasifiers; in stokers and fixed bed systems, such as updraft and downdraft gasifiers; in pressurized fluidized bed boilers and gasifiers; and in entrained flow reactors.

There is also a growing interest in co-combustion and co-gasification applications in which biomass and waste could be used together with fossil fuels in conventional pulverized-fuel boilers and more advanced systems. Integrated-gasification-combined-cycle boilers, supercritical combustion boilers, and entrained flow gasification reactors are examples of advanced systems in which biomass and waste materials can be mixed with fossil fuels up to 40% on an energy basis. There is also strong interest in fast and slow pyrolysis applications for the production of bio-oils and solid char that could be used as an advanced energy carrier.

Table 1-1 presents the operating characteristics of the temperature and pressure of the main reactors that are used today for the production of energy and fuels.

Table 1-1
Operating characteristics of boilers and gasifiers for energy and fuel production

Thermochemical Conversion Process	Operating Pressure (bars)	Operating Temperature (°C)
Atmospheric combustion/gasification	1	900
Atmospheric combustion/gasification	1	1300
Supercritical combustion/oxyfuel combustion	1	1600+
Pressurized combustion/gasification	2–50	1000
High-temperature pressurized gasification	2–50	1600
Pyrolysis production of bio-oil/char	1	600

As seen from Table 1-1, pyrolysis applications have the lowest temperature and pressure requirements, but the produced bio-oil/char has to be almost free of alkali metals, chlorine, and sulfur to ensure its stability and thermal behavior during its later utilization in combustion and gasification applications.

Atmospheric combustion and gasification can be divided into three main categories according to the operating temperature. Of these three categories, the first one, where the operating temperature is limited to 900°C, is mainly used for small-scale energy and fuel production. The second category, where the temperature is limited to 1300°C, is mainly used today for large-scale energy production. The third category, where the operating temperature is limited to 1600°C, constitutes the future regarding large-scale, high-conversion-efficiency energy production.

Pressurized combustion and gasification can be divided into two main categories. The first category, where the operating temperature is limited to 900°C, is commercial today regarding combustion, and it is in the demonstration phase regarding gasification. It is used mainly for energy and, to a smaller degree, fuel production. The second category, where the operating temperature is limited to 1600°C, is currently in the demonstration phase at a few commercial plants (in the case of combustion) and the subject of a few large-scale demonstrations (in the case of gasification). It is considered the technology of tomorrow for energy and fuel production.

All of these technologies, regardless of their commercial status, currently use very few low-quality biomass and waste materials as firing or co-firing feedstock. This is because of the significant ash-related problems associated with these low-quality materials in large volumes.

Figures 1-1 and 1-2 present the recommended minimum removal rate targets for the leaching process when using low-cost biomass and waste materials as feedstock for the production of energy and fuels in large scale for the different conversion technologies. The basis for these recommendations is extensive laboratory-scale and pilot-scale testing performed during the last 15 years using various combustors and gasifiers operating at temperatures as high as 1300°C and pressures as high as 40 bars and a thorough study and understanding of the composition and properties of many low-cost biomass and waste material.

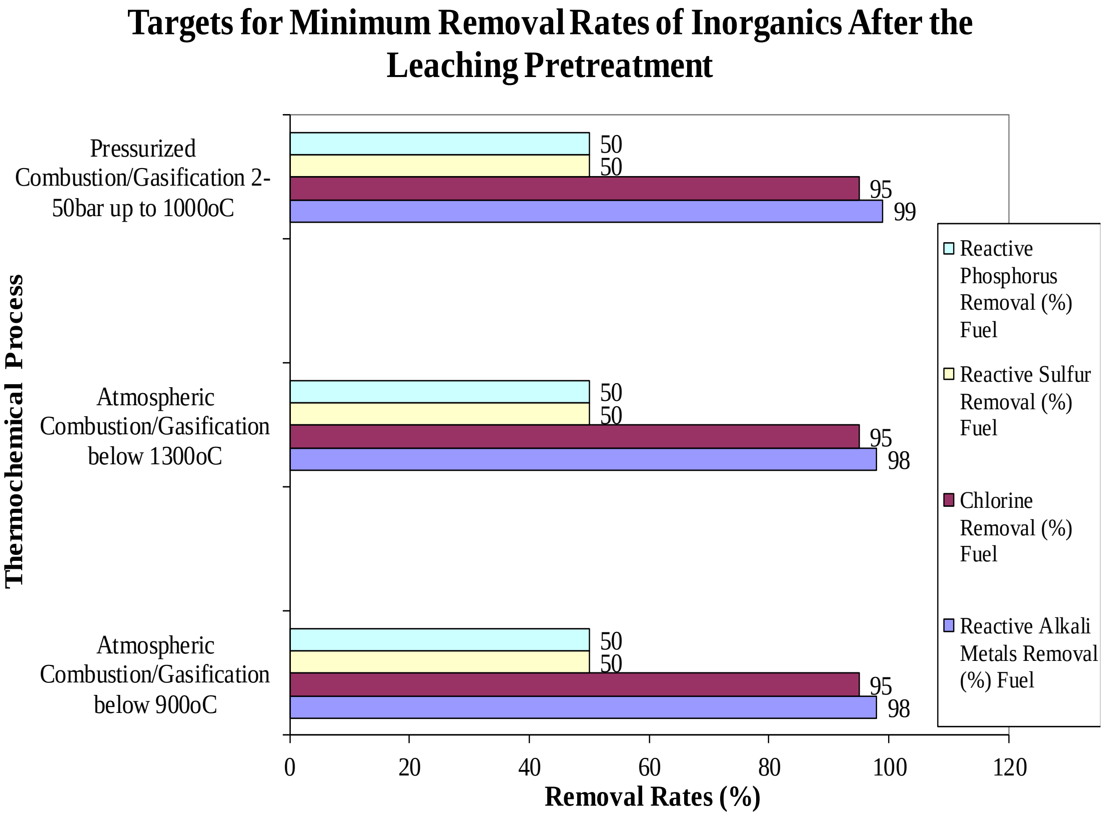

Figure 1-1
Targets for minimum removal rates of inorganics after the leaching pretreatment: thermochemical processes

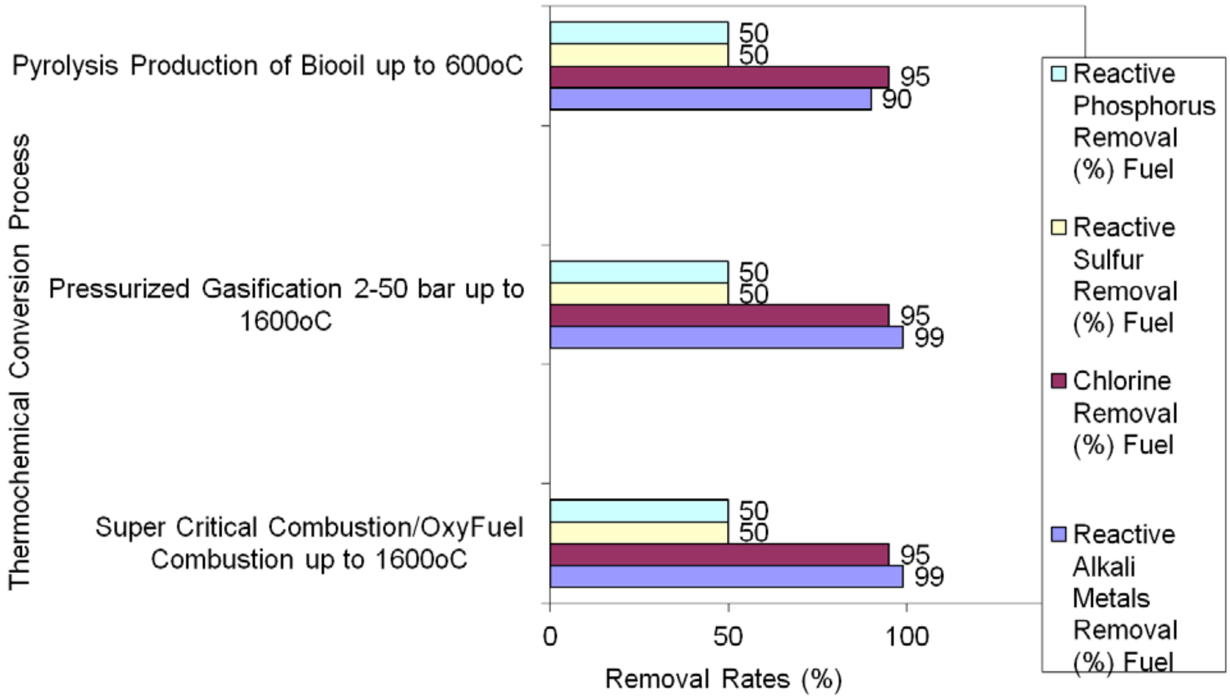

Figure 1-2
Targets for minimum removal rates of inorganics after the leaching pretreatment: thermochemical conversion processes

As seen from Figures 1-1 and 1-2, the most important condition to target is the presence of chlorine, which must be almost completely removed to substantially reduce or eliminate the ash-related problems arising from the use of biomass and waste materials. The role of chlorine in the inorganic transformations during thermochemical conversion was explained in Section 1.2.

The second objective is the removal of the reactive forms of alkali metals, in percentages higher than 99% for combustion and gasification applications and at least higher than 90% for bio-oil production. Finally, the reactive forms of phosphorus and sulfur in low-quality biomass and waste materials should be reduced to below 50% from the amount present in the raw feedstock.

Although heavy metals are not included in the preceding targets, our recommendation is that, for metals such as zinc and lead, the removal rates be similar to those proposed for alkali metals. However, for metals such as copper, cadmium, and nickel, the removal rates should be similar to those proposed for phosphorus and sulfur.

1.6 Properties of Raw Biomass Compared to Leached Biomass

Table 1-2 presents the best estimates of the ranges of the main properties of the leached biomass versus the original, untreated biomass for the main contaminants of interest. These properties can vary, depending on the type of the biomass materials, solvents used for the leaching pretreatment, and any additional special properties and characteristics that we would like to give them to maximize or minimize some of their effects on energy conversion systems.

Table 1-2
Main properties of raw versus leached biomass

Thermochemical Conversion Process	Original Biomass	Leached Biomass
Ash content	100%	-80%/+10%
High heating value (HHV)	100%	5–20%
Chlorine content	100%	-99%
Reactive alkali metals content	100%	-99%
Reactive sulfur content	100%	-50%
Reactive phosphorus content	100%	-50%

In 2010, Thermorefinery Technologies partnered with the Electric Power Research Institute (EPRI) to investigate more thoroughly the effects of its proprietary leaching technology in the upgrading of various difficult biomass materials to produce clean (alkali and chlorine-free) biomass fuels. As part of this endeavor, EPRI sponsored, through its Program on Technology Innovation, an extensive set of bench-scale tests using biomass feedstock and agricultural waste materials to optimize and assess the potential of this innovative leaching pretreatment technology.

Tests proved that the innovative leaching technology works efficiently in all cases for all of the different biomass and waste materials. Different solvents were specifically designed to maximize the effect of the leaching technology on specific biomass materials. For all of the feedstock tested, the content of reactive alkali metals in the leached products was reduced by more than 90%, chlorine by more than 99%, and sulfur and phosphorus 30–80%. Ash's melting points were seen to increase in a range of 400–800°C, depending on the solvents used and the specific biomass material. The results of this work were published in the EPRI report *Program on Technology Innovation: Biomass Leaching Pre-Treatment Technology Bench Testing* (1022720).

Section 2: Scope of Work and Testing Methods

2.1 Scope of Work

The project's main objective was to generate more leaching data from additional agricultural residue biomass materials. The new data was used to upgrade the leaching process Aspen Plus[4] model and develop coefficients that can be used to predict the leaching behavior of additional agricultural residue biomass materials. During this project, limited modeling activities and experimental work were performed.

Most of the work was to analyze and test three additional agricultural residues/grasses—corn stover, barley straw, and miscanthus—to generate additional data to upgrade the leaching model and create coefficients that will be able to predict the leaching behavior of additional agricultural biomass. All of these biomass materials belong to the high-silica biomass feedstock category.

The specific objectives of this bench-scale project were as follows:

- Limited testing of various biomass feedstock materials to increase the number of biomass materials included in the model's database. In total, 15 pretreated (leached) and 3 original biomass samples were analyzed and tested.
- Application of the experimental results in the Aspen Plus model.
- Publication of the final report on the modeling and experimental activities performed during the project.

2.2 Testing Facility and Process Description

The leaching tests applying both the general testing procedure and the special testing procedure took place at the Laboratory of Organic and Environmental Technologies at the School of Chemical Engineering of the National Technical University of Athens (Greece). Some of the analysis and characterization work regarding pH, electrical conductivity, mass loss, moisture, ash content, and sintering tests took place in the same laboratory.

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[4] Aspen Plus is a registered trademark of Aspen Technology, Inc.

Most of the analysis and characterization work of the original untreated biomass materials as well as that after the leaching tests was performed at the Institute of Geology and Mineral Exploration (www.igme.gr) in Athens, Greece. Analyses performed there included ash elemental analysis, proximate and ultimate analysis, chlorine determination, and gross calorific value.

Both facilities apply International Organization for Standardization (ISO) testing procedures to guarantee the validity of the test results.

The biomass materials selected were used to perform various leaching tests. The testing procedures, equipment, and sequence are described in Section 2.5. Details of the different conditions are presented in Table 2-1.

Table 2-1
Tests to be performed during the testing program

Biomass Leaching Tests	Corn Stover	Barley Straw	Miscanthus	Number of Tests
Solvent 1*	X	X	X	6
Solvent 2*	X	X	X	6
Pure water*	X	X	X	3
Particle size 1	X	X	X	
Temperature 1 (T1)	X	X	X	
Contact time 1 (t1)	X	X	X	
Solvent concentration 1(C1)	X	X	X	
Solvent concentration 2 (C2)	X	X	X	
Number of tests	5	5	5	15

*See Section 2.4.

2.3 Biomass Feedstock

The following three biomass materials have been used in the testing performed during the EPRI Program on Technology Innovation project:

- Corn stover
- Barley straw
- Miscanthus

These biomass materials represent abundant, difficult agricultural residues and energy crops with the potential to be used for energy production in traditional power plants. Approximately 5–10 kg of dry matter were used from each biomass material as the base sample to run all of the leaching/prewashing tests. All of the materials were air-dried and kept in sealed plastic bags to ensure that the material would not undergo any kind of biological degradation or moisture uptake while the biomass leaching tests were performed. In this way, we made sure that the raw materials used in the tests had constant composition and properties.

The biomass samples were milled in a particle size below 2 mm before they were used in the leaching process. Miscanthus leached most easily, followed by corn stover and barley straw. Barley straw was the most difficult. The initial corn stover material received had a large volume of extraneous material (soil and rocks) due to its storage conditions. As a result, the ash content of corn stover was quite high (>30% dry basis). The miscanthus biomass was very wet as received (>70% moisture content) because the harvesting period was in November.

2.4 Analytical Methods: Solvents Used

Different solvents were used during the project's leaching tests. Solvent 1 was of a basic nature, and Solvent 2 was of an acidic nature.

Leaching tests were also performed with deionized water for comparison. Deionized water was used to prepare the solvent solutions for the various leaching tests. The solutions had a concentration of 0.5% and 2% weight per volume (w/v) in solvent for all of the laboratory tests.

For all of the samples treated under the general and special set of conditions, the following analysis and characterization were applied:

- Moisture determination
- Ash determination
- pH
- Ion conductivity
- Ash sintering test in a muffle furnace up to 1100°C
- Mass loss
- Ash analysis by inductively coupled plasma (ICP) spectroscopy (SiO_2, Al_2O_3, TiO_2, Fe_2O_3, CaO, MgO, Na_2O, K_2O, P_2O_5, SO_3)
- The fuel's fouling potential index (kg [K_2O+Na_2O]/GJ)
- Elemental analysis (CHNSO)
- Determination of gross calorific value
- Biomass chlorine content
- Proximate analysis (ash, volatiles, fixed carbon)
- Chemical oxygen demand (COD) in the leachates

No further leachate analysis, apart from the COD determination, was performed because it was not necessary in order to achieve the targets of the project. Also, the funds available were limited.

The following ASTM International and ISO analytical methods were used to analyze and characterize the biomass, ash, and liquid samples:

- Moisture-Ash, ASTM D1102-84 (reapproved 1990)
- Volatiles, ASTM D3175-89a (reapproved 1993)
- Ultimate Analysis (CHN), ASTM D5373
- Ultimate Analysis (S), ASTM D4239
- Gross Calorific Value, ASTM D2015-95
- Chlorine Analysis, ASTM D4208
- Ash Elemental Analysis, ASTM D3682

2.5 General Testing Procedure

This section describes the procedures followed during the different tests performed in this research project.

The leaching process took place in a batch laboratory-scale mode using the following equipment and sequence:

1. Glass beakers of 2-l and 4-l volume were used to perform the leaching/prewashing tests.
2. A mechanical stirrer agitated the samples at a stirring rate of 5000 rpm.
3. The liquid solution was formed by mixing the water with the water-soluble solvents. The temperature of the solution was 20°C.
4. The biomass material was soaked into the glass container after the liquid solution reached the right temperature and was pretreated for the specific period required by the process conditions.
5. Before the start and at the end of the pretreatment process, the liquid pH and ion conductivity were determined.
6. The slurry was emptied into a plastic net with 200-µm openings, from which the liquid was squeezed out using manual force.
7. The solid residue was left to dry in the open air after this process.
8. The collected leachate was vacuum-filtered to collect the small biomass particles escaping from the filter press, and some of it was kept for COD determination.
9. After every leaching/prewashing test, the glass beakers were cleaned with soap and rinsed with deionized water so that they were ready to be used again for another test. Similar cleaning was applied to all of the testing equipment and devices that could become contaminated, be used in a different test, or be used with another material.

Three to four leaching/prewashing tests were performed daily on an 8-hour shift to ensure that there would be enough time to meet all of the quality specifications required to guarantee valid test results.

All of the samples analyzed were kept in small sealed plastic bags with adhesive tags where the code name of each sample was written. An Excel[5] spreadsheet was prepared. It included data on all of the analyzed samples with identification codes for each of the conditions used for leaching/prewashing tests. This spreadsheet was updated weekly to include all of the leaching/prewashing tests and the results from the different analytical tests for each biomass sample.

Table 2-1 presents the number of biomass leaching/prewashing tests performed during the Program on Technology Innovation project. A total of 15 biomass pretreatment tests were scheduled. Table 2-1 presents the test matrix for the leaching/prewashing tests during the testing program. As seen from Table 2-2, 12 leaching tests were performed with the different solvents. In addition, three more tests (one test per material) were performed as references to compare leaching performance improvement when using specifically engineered solvents. In total, we performed 15 leaching tests.

Table 2-2
Test matrix for the leaching/pre-washing tests with solvents during the testing program

Biomass Type	**Number of Tests with Solvent 1 in Pure Deionized Water**		**Number of Tests with Solvent 2 in Pure Deionized Water**		**Total Number of Tests**
	Solvent Concentration C1	**Solvent Concentration C2**	**Solvent Concentration C1**	**Solvent Concentration C2**	
Corn stover	1	1	1	1	4
Barley straw	1	1	1	1	4
Miscanthus	1	1	1	1	4

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[5] Excel is a registered trademark of Microsoft Corp.

Section 3: Results and Discussion from the Leaching Tests and Modeling Activities

3.1 Leaching Tests

Tables 3-1 to 3-3 present the basic conditions applied during the leaching tests performed with the different biomass materials.

Table 3-1
Conditions applied during the corn stover leaching process

Biomass Samples	Solvent Type	Solvent Concentration (%w/v)	Leaching Period (min)	Leaching Temperature (°C)	Solid/Liquid Ratio (%), Dry Basis	Water Type	Agitation Speed (rpm)
Corn 1	None	None	t1	T1	R1	Deionized	600
Corn 2	Solvent 2	C1	t1	T1	R1	Deionized	600
Corn 3	Solvent 2	C2	t1	T1	R1	Deionized	600
Corn 4	Solvent 1	C1	t1	T1	R1	Deionized	600
Corn 5	Solvent 1	C2	t1	T1	R1	Deionized	600

Table 3-2
Conditions applied during the barley straw leaching process

Biomass Samples	Solvent Type	Solvent Concentration (%w/v)	Leaching Period (min)	Leaching Temperature (°C)	Solid/Liquid Ratio (%), Dry Basis	Water Type	Agitation Speed (rpm)
Barley 1	None	None	t1	T1	R2	Deionized	600
Barley 2	Solvent 2	C1	t1	T1	R2	Deionized	600
Barley 3	Solvent 2	C2	t1	T1	R2	Deionized	600
Barley 4	Solvent 1	C1	t1	T1	R2	Deionized	600
Barley 5	Solvent 1	C2	t1	T1	R2	Deionized	600

Table 3-3
Conditions applied during the miscanthus leaching process

Biomass Samples	Solvent Type	Solvent Concentration (%w/v)	Leaching Period (min)	Leaching Temperature (°C)	Solid/Liquid Ratio (%), Dry Basis	Water Type	Agitation Speed (rpm)
Miscanthus 1	None	None	t1	T1	R3	Deionized	600
Miscanthus 2	Solvent 2	C1	t1	T1	R3	Deionized	600
Miscanthus 3	Solvent 2	C2	t1	T1	R3	Deionized	600
Miscanthus 4	Solvent 1	C1	t1	T1	R3	Deionized	600
Miscanthus 5	Solvent 1	C2	t1	T1	R3	Deionized	600

As seen from Tables 3-1 through 3-3, similar conditions applied in most cases during the leaching tests. In specific, each biomass material was leached using deionized water at T1 temperature for t1 time and was agitated using an IKA RW 20 Digital Dual-Range Mixer, 1/25- horsepower, 115-V mechanical agitator. The solid-to-liquid ratio used varied from R1% to R3% dry basis, depending on the biomass material.

Full analysis and characterization were conducted for the solids resulting from the leaching tests and the original biomass materials, whereas for the leachates, analysis was limited to pH, ion conductivity, and COD.

Tables 3-4 to 3-9 present the analysis and characterization of the three original biomass materials, their leached samples, and their ash.

Table 3-4
Analysis and characterization of original and pretreated corn cob biomass samples

Biomass Samples	**Corn Stover**	**Corn 1**	**Corn 2**	**Corn 3**	**Corn 4**	**Corn 5**
Proximate analysis (% dry basis)						
Moisture	5.23	6.73	11.85	11.93	7.08	8.96
Ash	32.90	28.61	25.73	16.01	18.19	12.10
Volatiles	60.46	71.14	73.14	74.71	74.23	74.66
Fixed carbon	6.64	0.25	1.13	9.28	7.58	13.24
Elemental analysis (% dry basis)						
Nitrogen	0.70	0.65	0.62	0.59	0.61	0.60
Carbon	35.81	43.43	44.41	44.87	44.89	45.51
Hydrogen	5.10	5.22	5.35	5.50	5.30	5.40
Sulfur	0.12	0.10	0.08	0.11	0.09	0.09
Chlorine	0.88	<0.01	<0.01	<0.01	<0.01	<0.01
Oxygen	24.49	21.99	23.81	32.92	30.92	36.30
HHV (MJ/kg)	12.99	16.22	16.73	17.47	16.95	16.57

Table 3-5
Analysis and characterization of original and pretreated barley straw biomass samples

Biomass Samples	**Barley Straw**	**Barley 1**	**Barley 2**	**Barley 3**	**Barley 4**	**Barley 5**
Proximate analysis (% dry basis)						
Moisture	3.39	8.84	8.65	7.72	9.29	7.10
Ash	8.20	5.96	5.06	4.55	5.94	7.34
Volatiles	74.95	77.08	78.86	78.73	78.71	78.64
Fixed carbon	16.86	16.96	16.08	16.72	15.35	14.02
Elemental analysis (% dry basis)						
Nitrogen	0.60	0.55	0.47	0.43	0.45	0.42
Carbon	43.03	44.58	46.04	45.32	44.81	44.10
Hydrogen	5.70	5.85	5.90	5.95	5.88	5.90
Sulfur	0.19	0.17	0.09	0.03	0.14	0.14
Chlorine	0.37	<0.01	<0.01	<0.01	<0.01	<0.01
Oxygen	41.91	42.89	42.44	43.72	42.78	42.10
HHV (MJ/kg)	18.12	18.57	18.86	19.05	18.89	18.53

Table 3-6
Analysis and characterization of original and pretreated miscanthus biomass samples

Biomass Samples	**Miscanthus**	**Miscanthus 1**	**Miscanthus 2**	**Miscanthus 3**	**Miscanthus 4**	**Miscanthus 5**
Proximate analysis (% dry basis)						
Moisture	30.25	12.86	9.49	9.26	8.95	9.55
Ash	3.05	3.08	2.93	2.86	3.41	4.89
Volatiles	77.95	79.92	80.21	80.11	80.02	79.26
Fixed carbon	19.00	17.00	16.86	17.03	16.57	15.85
Elemental analysis (% dry basis)						
Nitrogen	0.60	0.50	0.46	0.40	0.43	0.41
Carbon	46.14	47.17	47.60	46.84	47.20	47.16
Hydrogen	6.00	6.20	6.30	6.35	6.30	6.40
Sulfur	1.05	0.95	0.55	0.36	0.79	0.78
Chlorine	0.22	<0.01	<0.01	<0.01	<0.01	<0.01
Oxygen	42.94	42.10	42.16	43.19	41.87	40.36
HHV (MJ/kg)	18.98	19.99	19.93	19.79	19.85	19.71

Table 3-7
Ash elemental analysis using inductively coupled plasma optical emission spectroscopy (ICP-OES) of original and pretreated corn cob biomass samples

Biomass Samples	**K_2O**	**Na_2O**	**SiO_2**	**Al_2O_3**	**Fe_2O_3**	**CaO**	**MgO**	**P_2O_5**	**SO_3**	**LOI**	**Cl**
Corn stover	2.87	0.40	18.16	2.28	0.73	4.24	1.31	0.30	0.28	2.01	0.88
Corn 1	0.60	0.39	17.22	2.95	0.97	3.55	0.51	0.09	0.07	1.54	0.01
% Difference	-78.92	-4.44	-5.16	29.14	32.40	-16.25	-61.07	-68.11	-73.81	-23.27	-98.86
Corn 2	0.58	0.25	17.29	2.41	0.74	2.07	0.48	0.10	0.07	0.78	0.01
% Difference	-79.86	-38.98	-4.79	5.48	0.91	-51.21	-63.35	-67.41	-73.66	-61.15	-98.86
Corn 3	0.44	0.30	10.99	1.66	0.54	1.00	0.30	0.08	0.06	0.31	0.01
% Difference	-84.78	-26.74	-39.48	-27.47	-26.54	-76.41	-76.99	-74.45	-78.37	-84.65	-98.86
Corn 4	0.62	0.34	11.84	1.46	0.44	2.49	0.33	0.07	0.07	0.09	0.01
% Difference	-78.37	-16.76	-34.80	-35.97	-40.07	-41.35	-74.55	-77.42	-74.30	-95.39	-98.86
Corn 5	0.40	0.16	6.44	0.72	0.22	2.66	0.22	0.05	0.06	1.16	0.01
% Difference	-86.02	-61.20	-64.55	-68.53	-69.63	-37.32	-83.38	-84.68	-79.89	-42.43	-98.86

Table 3-8
Ash elemental analysis using ICP-OES of original and pretreated barley straw biomass samples

Biomass Samples	**K_2O**	**Na_2O**	**SiO_2**	**Al_2O_3**	**Fe_2O_3**	**CaO**	**MgO**	**P_2O_5**	**SO_3**	**LOI**	**Cl**
Barley straw	0.64	0.20	4.60	0.26	0.07	1.00	0.18	0.14	0.22	0.75	0.37
Barley 1	0.32	0.12	4.06	0.11	0.04	0.76	0.12	0.08	0.14	0.28	0.01
% Difference	-49.36	-41.91	-11.74	-58.89	-50.37	-23.68	-32.68	-40.89	-34.16	-62.33	-97.29
Barley 2	0.18	0.08	4.00	0.08	0.03	0.43	0.08	0.08	0.08	0.08	0.01
% Difference	-71.66	-60.41	-13.07	-68.74	-52.97	-56.69	-58.85	-46.59	-63.31	-89.11	-97.29
Barley 3	0.14	0.06	3.69	0.11	0.04	0.29	0.06	0.07	0.08	0.05	0.01
% Difference	-78.62	-70.13	-19.86	-58.48	-40.97	-70.69	-67.52	-53.66	-62.08	-93.07	-97.29
Barley 4	0.13	0.04	3.64	0.09	0.04	1.31	0.09	0.08	0.13	0.48	0.01
% Difference	-79.23	-80.90	-20.82	-65.01	-50.54	31.33	-49.54	-44.86	-41.69	-35.47	-97.29
Barley 5	0.16	0.09	4.20	0.13	0.06	2.29	0.09	0.08	0.11	0.09	0.01
% Difference	-75.65	-55.23	-8.70	-49.90	-16.14	129.11	-49.39	-42.77	-49.54	-88.13	-97.29

Table 3-9
Ash elemental analysis using ICP-OES of original and pretreated miscanthus biomass samples

Biomass Samples	**K_2O**	**Na_2O**	**SiO_2**	**Al_2O_3**	**Fe_2O_3**	**CaO**	**MgO**	**P_2O_5**	**SO_3**	**LOI**	**Cl**
Miscanthus	0.15	0.01	2.31	0.01	0.01	0.29	0.12	0.04	0.03	0.06	0.22
Miscanthus 1	0.08	0.02	2.52	0.00	0.00	0.27	0.05	0.02	0.02	0.03	0.01
% Difference	-48.43	85.68	8.86	-74.22	-63.93	-4.44	-54.35	-39.98	-40.70	-56.50	-95.50
Miscanthus 2	0.05	0.01	2.58	0.00	0.00	0.17	0.07	0.02	0.02	0.02	0.01
% Difference	-65.03	-0.84	11.45	-79.56	-65.69	-40.78	-37.96	-53.45	-48.07	-70.44	-95.50
Miscanthus 3	0.06	0.02	2.48	0.01	0.01	0.13	0.05	0.01	0.02	0.02	0.01
% Difference	-63.87	56.84	7.44	-32.17	-33.02	-52.83	-58.42	-65.29	-47.47	-69.22	-95.50
Miscanthus 4	0.07	0.03	2.42	0.00	0.01	0.63	0.08	0.02	0.02	0.15	0.01
% Difference	-57.71	113.72	4.87	-85.73	-44.10	121.94	-32.61	-43.57	-25.28	157.43	-95.50
Miscanthus 5	0.07	0.02	2.67	0.00	0.01	1.59	0.11	0.02	0.02	0.34	0.01
% Difference	-52.62	53.24	15.49	-93.18	-42.74	455.51	-10.26	-48.75	-36.97	467.31	-95.50

From Table 3-4, corn stover is seen to have very high ash content due to its storage conditions that contaminated it with soil. As a result, the sample had some homogeneity issues, and the ash content of the leached corn stover samples was lower than the original untreated material but still significant.

According to Table 3-7, leaching has a very positive effect regarding the amounts of chlorine, sulfur, phosphorus, and alkali metals contained in the ash of the original untreated corn stover. All of these elements were substantially reduced or eliminated during the pretreatment process.

As shown in Figure 3-1, the fouling potential index is also reduced significantly after the leaching process, but it is higher than 0.17, considered to be the limit for fouling behavior for coal ash. However, the complete elimination of chlorine and reactive alkali metals from the ash of the leached samples has transformed the specific samples to nonfouling materials, as the ash sintering tests confirmed.

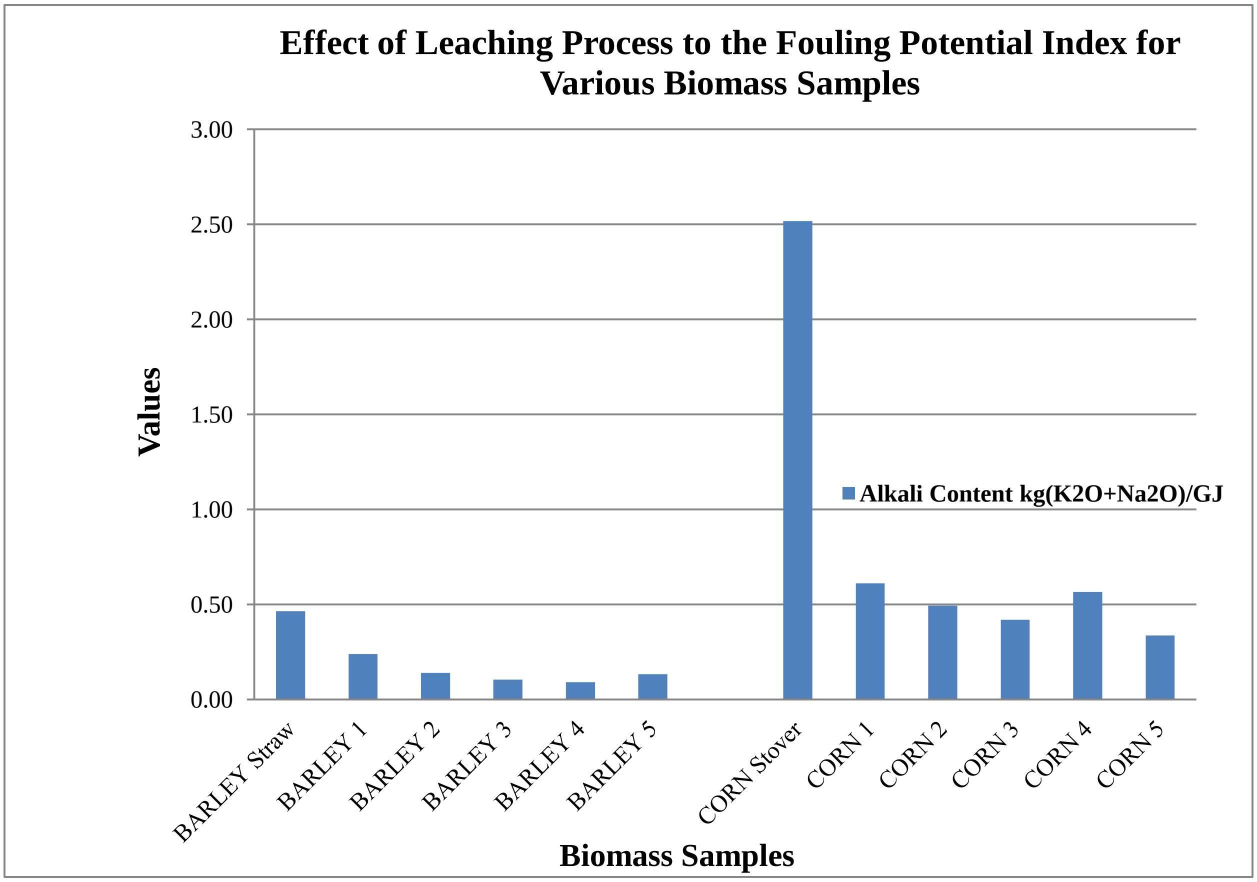

Figure 3-1
Effect of leaching process on the fouling potential index for corn stover and barley straw biomass samples

Tables 3-5 and 3-8 present the results from the analysis and characterization of barley straw samples and their ash. Again, the leaching process had a very positive effect regarding the main characteristics of the barley straw biomass, such as its volatiles, calorific value, sulfur content, and ash composition. Again, the use of solvents eliminated all chlorine and removed substantial amounts of alkali metals, sulfur, and phosphorus, transforming the barley straw biomass into a clean biomass ready to be used in combustion and gasification applications without ash-related problems. Figure 3-1 shows that the fouling index is also substantially reduced after the leaching process to below the 0.17 value in all cases, when a solvent, not just deionized water, is used for the leaching process. The results from the sintering tests also verify that the ash derived from leached samples does not melt below 1100°C.

Finally, the biomass materials with the highest initial moisture, chlorine, and volatiles content and the lowest ash compared to the other two biomass materials were analyzed. The data in Tables 3-6 and 3-9 show that the leaching process had the same positive effects on this material as in the case of the other two biomass materials analyzed.

According to Figure 3-2, the fouling index was reduced by more than 50% after the application of the leaching process, and miscanthus showed the lowest fouling index compared to the other two biomass materials.

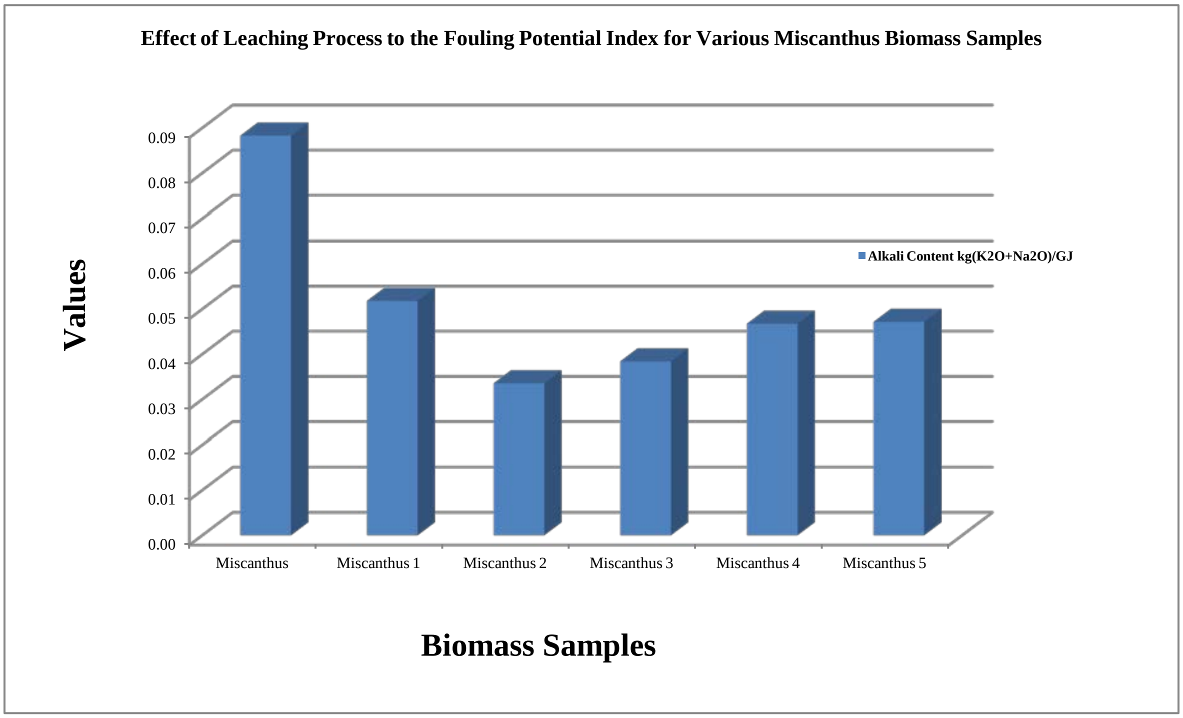

Figure 3-2
Effect of the leaching process on the fouling potential index for the miscanthus biomass samples

However, the reader has to be warned that, as indicated in previous EPRI reports (see, for example, report 1024662), the fouling index is not a trustworthy index to assess the fouling and melting tendency of a biomass ash. We calculate this index and present the relative results just for information purposes and always with the warning that the real behavior of the ash from the different biomass materials is, in many cases, quite different compared to the indications provided by the coal-based fouling index.

As the sintering tests show, the ash of the leached samples melts at temperatures higher than 1100°C when a solvent is used, compared to 800°C in the case of the untreated miscanthus biomass. Water leaching improves the ash behavior of the pretreated biomass. However, as found and documented before (see EPRI report 1024662), water leaching alone is not enough to guarantee the elimination of ash-related problems in high-alkali and chlorine agricultural biomass. Similar results were observed for the other two biomass materials.

Table 3-10 presents the results from the COD determination of the leachates. In Table 3-10, corn stover leachates show the highest COD values among the three biomass materials tested, followed by the barley straw leachates and the miscanthus.

Table 3-10
COD values of the different biomass leachates

Biomass Leachates	COD (mg/l)
Corn 1	5960
Corn 2	7180
Corn 3	18880
Corn 4	8980
Corn 5	12300
Barley 1	2350
Barley 2	3790
Barley 3	8650
Barley 4	3030
Barley 5	10050
Miscanthus 1	1860
Miscanthus 2	3640
Miscanthus 3	10200
Miscanthus 4	3350
Miscanthus 5	11880

3.2 Modeling Work

The new values regarding the examples of the three biomasses' pretreatment have been applied to the generic model for grasses, which is evaluated by experimental results for different solvent concentrations. The generic Aspen Plus model for grasses is first tested in terms of its ability to simulate the pretreatment process of additional biomass feedstocks without increasing the factors' range of the MECHDEW block and, consequently, the error coming from the model (difference between modeling and experimental results). Therefore, the range of the factors of the generic pretreatment model includes the case of miscanthus pretreatment because the factors given in the MECHDEW block of the Aspen Plus simulation tool are within the range of the factors applied for the generic model.

Moreover, the model has become more specific in terms of a narrower range of the MECHDEW block factors when applied to a new biomass feedstock, such as miscanthus. A new subcategory of the factors range has been added concerning miscanthus, thus making the range more accurate when the generic model for grasses is applied for the aforementioned biomass fuel.

Figure 3-3 presents the comparison between the experimental and modeling results for the composition of each ash compound (Si, Al, Fe, Ca, Mg, K, Na, SO_3, and P) at temperature T1 for three different Solvent 1 concentrations (C1, C2, and C3) in deionized water and two Solvent 2 concentrations (C2 and C3) in deionized water, respectively, when corn stover was used as biomass feedstock.

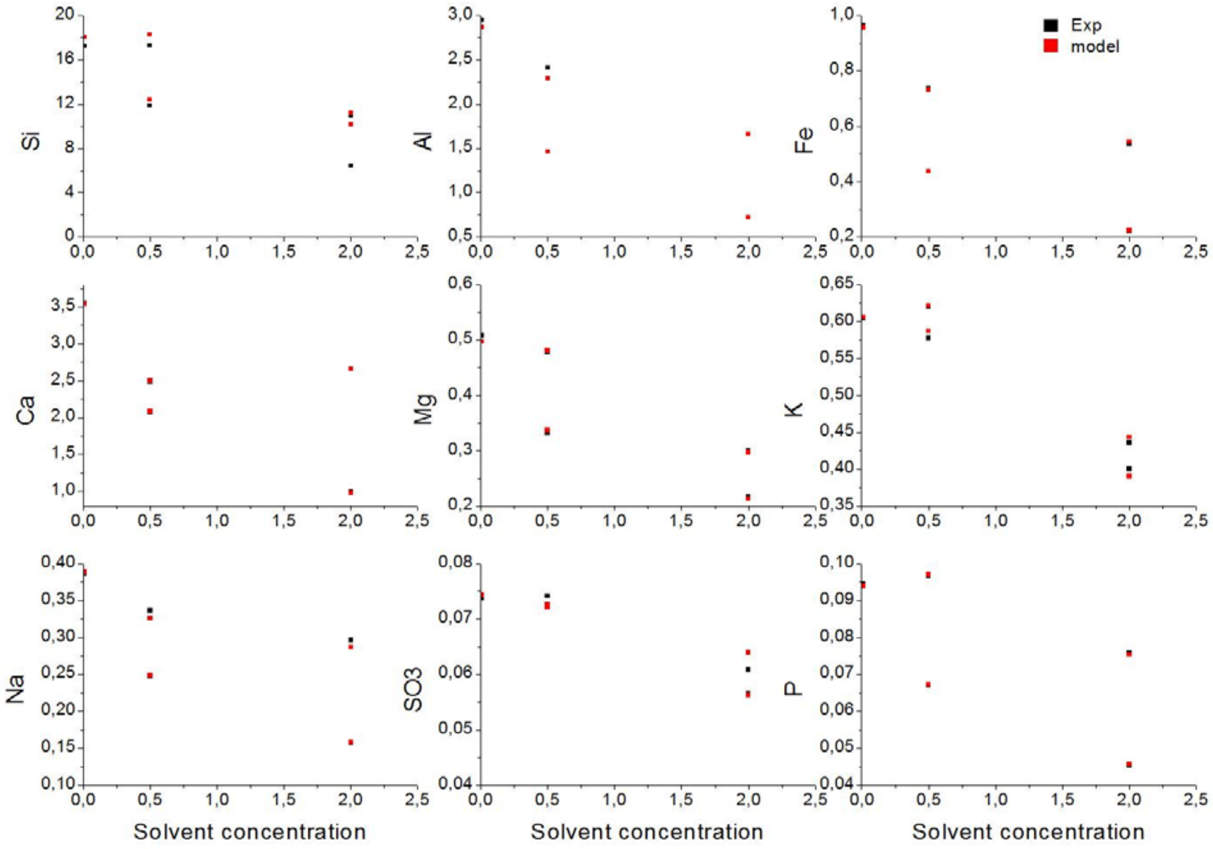

Figure 3-3
Comparison of the experimental and modeling results for corn stover at T1 for three different solvent concentrations (C1, C2, and C3)

As can be seen from Figure 3-3, the experimental and modeling results show a very good correlation to each other. The best fit is observed in the cases of Fe, Ca, Mg, K, Na, and P, where the experimental and modeling values are quite similar. In the cases of Si, Al, and SO_3, most values are also similar, and there are some differences in two or three cases for each element. As can be seen, regarding all of the ash compounds, the ash composition decreases or is approximately at the same level with increasing solvent concentration for both solvents.

Figure 3-4 shows the comparison of the experimental and modeling results for the composition of each ash compound (Si, Al, Fe, Ca, Mg, K, Na, SO_3, P) at the temperature of T1 for three different solvent concentrations (C1, C2, and C3)—Solvent 1 in deionized water and C2 and C3 Solvent 2 in deionized water, respectively, for barley straw as biomass feedstock.

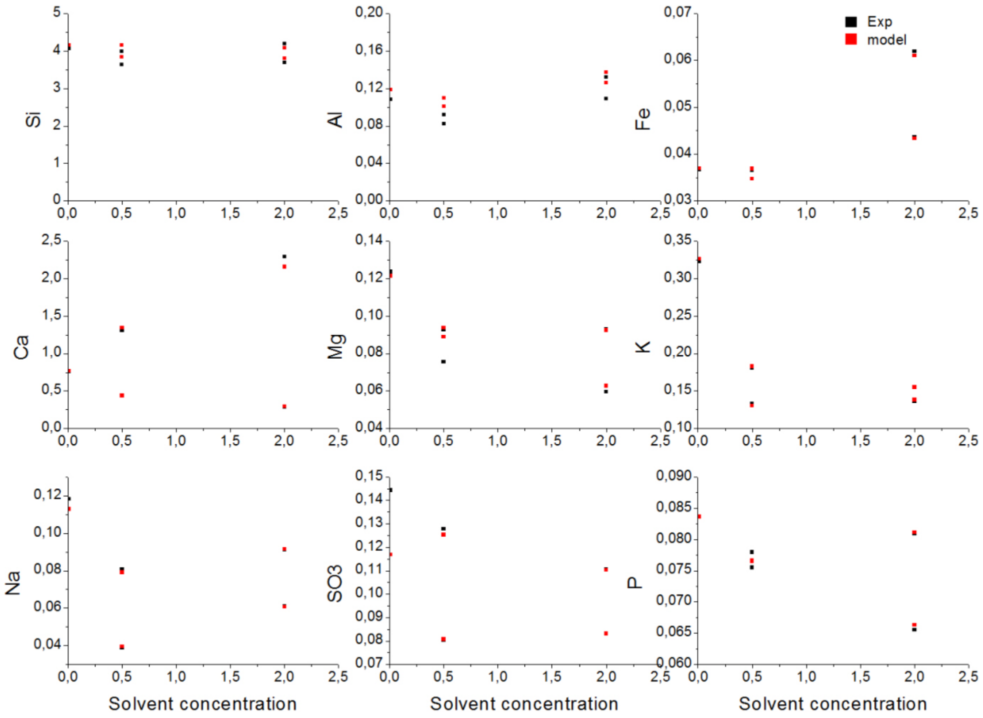

Figure 3-4
Comparison of the experimental and modeling results for barley straw at T1 for three different solvent concentrations (C1, C2, and C3)

According to Figure 3-4, the experimental and modeling results show a very good correlation to each other. The best fit is observed in the cases of Fe, Ca, Mg, K, Na, and SO_3, where almost all of the experimental and modeling values are very similar. In the cases of Si, Al, and P, most values are also very similar, although there are some differences, especially in the case of Si and Al. For all of the ash compounds, the ash composition decreases or is approximately at the same level with increasing solvent concentration for both solvents.

Figure 3-5 shows the comparison of the experimental and modeling results for the composition of each ash compound (Si, Al, Fe, Ca, Mg, K, Na, SO_3, P) at temperature T1 for three different solvent concentrations (C1, C2, and C3)—Solvent 1 in deionized water and C2 and C3 Solvent 2 in deionized water, respectively, when miscanthus is used as biomass feedstock.

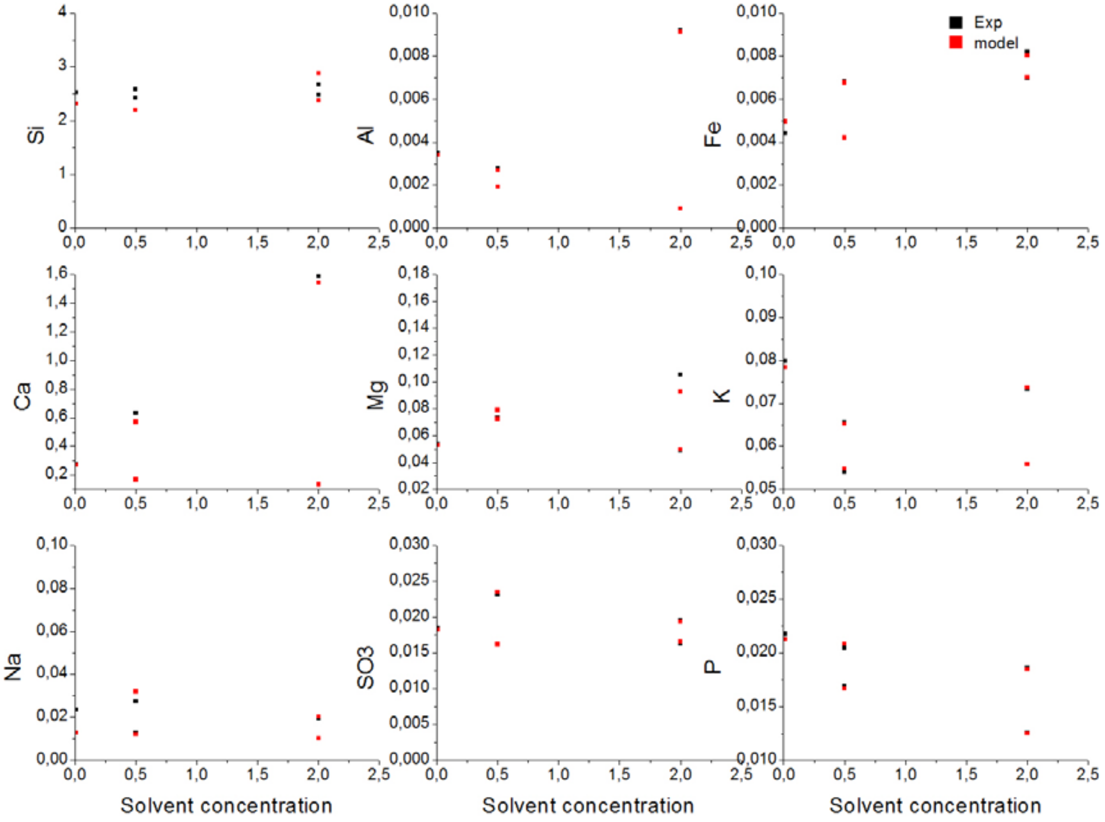

Figure 3-5
Comparison of the experimental and modeling results for miscanthus at T1 for three different solvent concentrations (C1, C2, and C3)

In Figure 3-5, the experimental and modeling results show a very good correlation to each other. The best fit is observed in the cases of Fe, Ca, Al, K, P, and SO3, where almost all of the experimental and modeling values are quite similar. In the cases of Si and Na, most values are also similar, although there are some differences, especially in the case of Si. For all of the ash compounds, the ash composition decreases or is approximately at the same level with increasing solvent concentration for both solvents.

To provide more emphasis on how a specific factor's range for each biomass feedstock influences the output of the generic model, an example applying the upper limit of the wheat straw factors' range in two previous cases of the generic model is depicted in Figure 3-6, where the maximum error that comes from the model is reduced after applying the new narrower factors' range and thus optimizing the leaching generic model for wheat straw.

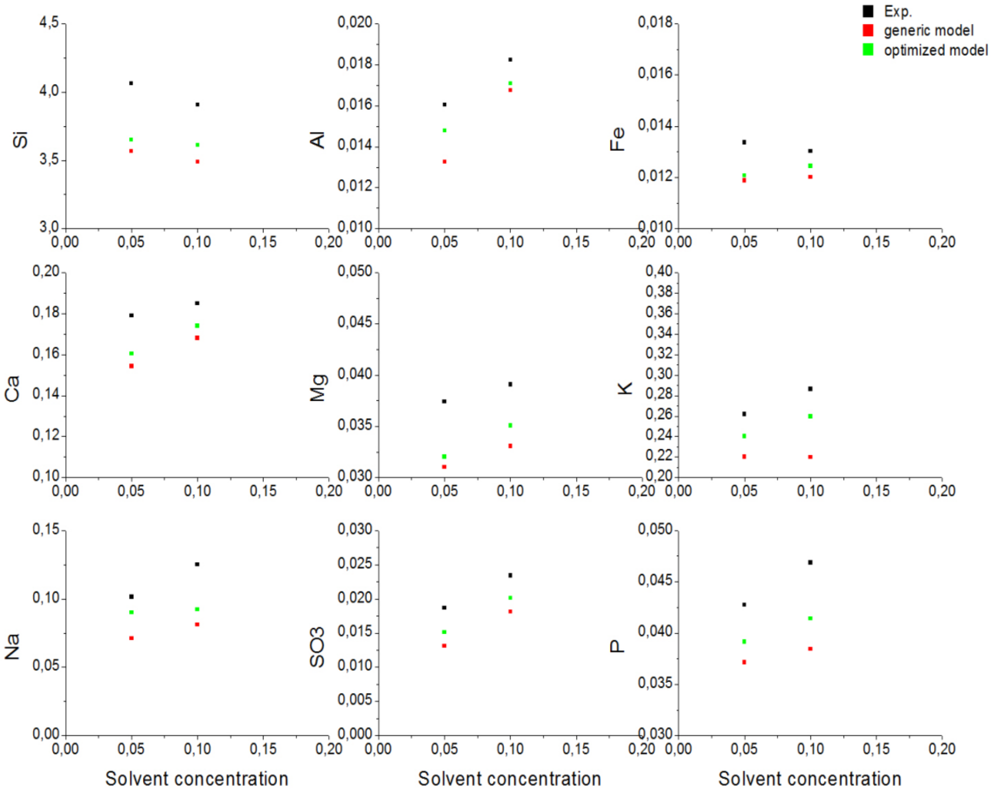

Figure 3-6
Comparison of the experimental and modeling results for wheat straw at T1 for three Solvent 1 concentrations (C1, C2, and C3) in deionized water and two Solvent 2 concentrations (R1 and R2) in deionized water

Section 4: Conclusions

4.1 Summary of Conclusions

The main findings of the laboratory-scale project are summarized as following:

- The leaching process had a very positive effect on each of the three biomass materials tested in this research, as we had seen in the previous experimental work performed in 2010 and 2011. This confirms that the Thermorefinery leaching process is a versatile process that can be applied to a wide range of biomass and waste materials with excellent results. Both solvents were fully suitable for the three types of biomass tested.
- The application of the new data points resulting from the analysis and characterization of the original biomass materials to the Aspen Plus leaching model developed in the frame of the EPRI-funded project (see *Program on Technology Innovation: Biomass Leaching Pre-Treatment Technology Bench Testing* [1022720]) had positive effects on the calculation of the model factors required to predict the behavior of the biomass materials through the leaching process. The additional data helped to narrow the range of values that the model factors take and, as a result, led to better estimation of the composition of the leached samples by the updated leaching model. The results presented in Figures 3-3 to 3-5 show an excellent match in most cases.
- Additional work will be needed, and more data have to be added to the leaching model to create factors that will reproduce the results from the leaching process with even higher accuracy, eliminating the need for experimental work and its associated costs.

- The application of the new data points to the case of wheat straw biomass, which had been analyzed during the research project executed in 2010–2011 (see *Program on Technology Innovation: Biomass Leaching Pre-Treatment Technology Bench Testing* [1022720]), shows that the new modeling results are better than those of the previous application of the Aspen Plus leaching model (see Figure 3-6).
- The update of the leaching model, which uses a combination of additional data from different biomass species and the introduction of reactions to accurately describe the leaching process, is expected to result in a useful tool. The updated model can be used to evaluate the leaching process alone or in combination with other processes, such as torrefaction, combustion, gasification, and pyrolysis, to evaluate the efficiency of the process and its integration into more complex processes.

4.2 Future Work

Future work might include an additional small research project in which modeling activities and limited experimental work will be performed. The main goal would be to further upgrade the existing leaching process model and increase the number of feedstocks in the model's database using the Aspen Plus model code. Post-upgrade, the model would be based on chemical reactions, compared to the simplistic mixing model used now.

Another area of possible future work involves using the Aspen Plus process economic analyzer to develop an integrated cost estimation of the leaching process. Limited experimental work will also be performed during this project to analyze and pretreat several additional feedstock materials to diversify the model's database and improve the reliability of its predictions.

Materials to be included will be decided and divided into three large categories, such as straws and grasses; woody biomass; and pits, kernels, and food waste. At least four to six different materials from each category would be analyzed, pretreated, and included in the database of the model.

The expected result of these projects would be a leaching model with the accuracy required to evaluate the leaching process in various scenarios as a standalone process as well as in combination with other processes—such as torrefaction, combustion, gasification, and pyrolysis—without the need to conduct experimental work.

The information derived from this updated model will assist significantly in the evaluation of complex cases and applications and will provide a valuable decision-making tool at a fraction of the cost of the experimental approach.

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