ABSTRACT

With an aging population of experienced coal scientists retiring there will be a reduction in our collective coal science communities ability at a time when the challenges facing coal are immense. This is particularly important in Illinois due to the large coal deposits and their economic importance. To better position the community to move forward in this time of transition a literature review, focused on Illinois coal was undertaken. The review captured the important observation of traditional fields, coking, solvent swelling, extraction, and gasification along with emerging areas such as application of microwave technology, molecular modeling and analysis advances, ionic solvents for extraction/fragmentation of coal, and the potential for sequestration of CO₂ within Illinois coals. The active and emerging academic research centers for coal science were determined both domestically, and internationally (with a focus on China) along with identification of areas of strength and specialization. The 200 plus page report (with 650 plus citations) cumulated with recommendations for Illinois coal science support for the next 5-10 years and recommendations for coal training opportunities. Specifically the reports address: sequestration in coal with a Illinois coal focus, gasification and char reactivity (Illinois coal focus), reactions with solvents and ionic liquids with Illinois coal and the nature of the extracts, microwave applications to coal (broad review), advances in molecular modeling and analytical techniques, a review of coking of Illinois coals and the current challenges, a review of the maceral and heterogeneity (with an Illinois coal focus), the active centers for coal science were determining both nationally (academic) and internationally with a special focus on the growth of Chinese coal research, indication on how the structure of Illinois coal (molecular representation) has utility in aiding specific conditions for feedstock (coal-to-chemicals), and recommendations for ICCI were produced.
EXECUTIVE SUMMARY

With an aging population of experienced coal scientists retiring there will be a reduction in our collective coal science communities ability at a time when the challenges facing coal are immense. This is particularly important in Illinois due to the large coal deposits and their economic importance. To better position the community to move forward in this time of transition a literature review, focused on Illinois coal was undertaken. The review captured the important observation of traditional fields, coking, solvent swelling, extraction, and gasification along with emerging areas such as application of microwave technology, molecular modeling and analysis advances, ionic solvents for extraction/fragmentation of coal, and the potential for sequestration of CO₂ within Illinois coals. The active and emerging academic research centers for coal science were determined both domestically, and internationally (with a focus on China) along with identification of areas of strength and specialization. The 200 plus page report (with 650 plus citations) cumulated with recommendations for Illinois coal science support for the next 5-10 years and recommendations for coal training opportunities. Specifically the reports address: sequestration in coal with a Illinois coal focus, gasification and char reactivity (Illinois coal focus), reactions with solvents and ionic liquids with Illinois coal and the nature of the extracts, microwave applications to coal (broad review), advances in molecular modeling and analytical techniques, a review of coking of Illinois coals and the current challenges, a review of the maceral and heterogeneity (with an Illinois coal focus), the active centers for coal science were determining both nationally (academic) and internationally with a special focus on the growth of Chinese coal research, indication on how the structure of Illinois coal (molecular representation) has utility in aiding specific conditions for feedstock (coal-to-chemicals), and recommendations for ICCI were produced.

We are in an era of funding challenges for the progression of basic and applied coal science during while the coal industry continues to face challenging times and considerable uncertainty. For the effective leveraging of Illinois Clean Coal Institute (ICCI) funding should be highly directed, serve the current and future needs of Illinois coal producers and Illinois-coal users. Thus, the institute needs to return to its roots both for new knowledge creation and ensuring a skilled workforce is in place to tackle issues of relevance to the Illinois coal extraction and users. This entails soliciting, encouraging and funding of “hands-on” coal research.
OBJECTIVES

Illinois coal has been well studied and despite economic downturns for two decades is again well situated to make a significant contribution to the energy security of the state and the nation. However, there is a significant challenge in experience and human capital. Many coal research centers have transformed into other focus areas during funding droughts and much of the talent in the field is now retired or close to retirement. To advance and to ensure progress is based on sound scientific principles, the proposal aims to generate documentation and peer-reviewed journal articles capturing the state-of-knowledge regarding the structure and behavior of Illinois basin coals, and where appropriate similar coals. This project broadly addressed the critical aspects of coal science with regard to structure and reactions occurring with: gasification and char reactivity (Illinois coal focus), reactions with solvents and ionic liquids with Illinois coal and the nature of the extracts, microwave applications to coal (broad review), advances in molecular modeling and analytical techniques, a review of coking of Illinois coals and the current challenges, a review of the maceral and heterogeneity (with an Illinois coal focus), the active centers for coal science were determining both nationally (academic) and internationally with a special focus on the growth of Chinese coal research, indication on how the structure of Illinois coal (molecular representation) has utility in aiding specific conditions for feedstock (coal-to-chemicals).

INTRODUCTION AND BACKGROUND

With an aging population of experienced coal scientists retiring there will be a reduction in our collective coal science communities ability at a time when the challenges facing coal are immense. This is particularly important in Illinois due to the large coal deposits and their economic importance. To better position the community to move forward in this time of transition a literature review, focused on Illinois coal, some relevant advances in processing (microwave treatments), analytical evaluation, molecular modeling, Illinois coal utilization (extraction, coking, maceral influences, and gasification), and CO2 sequestration in coal reviews were undertaken. Often the reports produced were focused on Illinois no. 6 Argonne Premium coal, the most well studied coal in existence, and other relevant coals when applicable. These documents collectively identify relevant literature and offer excellent starting points to address many of the challenges, historic and emerging, facing the utilization of Illinois coals in current or new markets.

EXPERIMENTAL PROCEDURES

This was a literature review project, traditional approaches were used to locate coal literature of relevance both specific to Illinois no. 6 (one of the Argonne Premium coals, and most well-studies coal in existence) and other relevant coals. To evaluate institutional contributions to coal science Articles containing “coal” in the title were identified using the ISI Web of Knowledge selecting only the Web of Science (Science Citation Index Expanded) database for English language publications between 1970 and 2010 (in the case of China also between 2000 and 2012) as one measure to identify those centers that have produced copious coal-related research (in English-language publications).
Knowledge tools were used to identify institutions and to parse those citations into an Endnote library. A customized bibliography style was created to examine titles and authors only within Microsoft Word. All of the text was converted into uppercase and the term coal removed using the find and replace tool prior to being uploaded into the Wordle software. The complexity of the cloud (based on article titles) communicates the breadth of information (here the subject area) with the leading visible words being the specialty or areas of focus for those institutions. For the coking report particular attention was paid to the historic circulars of the Illinois Geologic Survey.

RESULTS AND DISCUSSION

1. CO₂ SEQUESTRATION IN UNMINEABLE COAL SEAMS
Research was undertaken to identify, from the literature, the key issues and capacity estimations for CO₂ sequestration in unmineable Illinois coal seams. There has been interest in the coal community with copious experiments on powdered, cubed, and monoliths of coal, with and without confining stress and at various conditions. Field demonstrations have also furthered our understanding of the complex competing processes underway. The paper (Appendix A1) examines carbon dioxide sequestration in coal with an Illinois focus. The current state of knowledge and the uncertainties in the science are discussed, specifically addressing field demonstrations, methodology of capacity estimates, the role of applied stress and moisture in reducing the capacity, influence of mineral matter, pore size distribution determination by SAXS/SANS and its use, dynamic permeability, along with softening/rearrangement of the coal due to CO₂ exposure are addressed.

2. GASIFICATION REACTIONS AND CHAR REACTIVITY
The Illinois basin is a potential location for coal gasification with ample bituminous coal supplies, low coal transportation costs, an industrial base, and significant population to use electricity, liquid fuels, or coal-derived-chemicals. Gasification also has the advantage of easily dealing with the high sulfur content that historically limited Illinois coal use until scrubber systems had penetrated the coal utility fleet. Here the state of high heating-rate coal gasification knowledge relevant to Illinois coals is considered (Appendix A2). Thermoplasticity, as expected, was found to be sensitive to heating rate, pressure, and temperature. This in-turn influences reactivity with considerable reactivity differences being reported in the literature as conditions change. Mineral matter also appears to influence the extent of structural ordering of the char during conversion. Additives have also been shown to influence the thermoplastic transformations.

3. REACTIONS WITH SOLVENTS AND IONIC LIQUIDS AND THE NATURE OF THE EXTRACTS
In collaboration with Drs. Paul Painter and Caroline Burgess Clifford (Penn State) an extensive review considered the extent and kinetics of Illinois coal swelling, the solvent extraction yields (low and high temperatures) and nature of the extracts. The mechanism of swelling and extraction was discussed, including the recent ionic liquid work performed at Penn State. The implications for solvent studies involving Illinois no. 6 coal are in Appendix A3. Coal swelling factor was varied depending on solvent (and to a
lesser degree temperature) and ranged between 1 (non to low swelling for benzene) to 4.15 for tetrabutyl ammonium hydroxide. The swelling of Illinois coal has been explored using the standard tube height change approach, on surfaces, single particles, with pencil-like cores in dilatomatery experiments, and by NMR imaging. The kinetics of swelling was related to the network structure its relaxation process, and the bulkiness of the solvent. The overshoot and metastable state phenomena in coal swelling is observed for Illinois no. 6 coal. Coal extracts yields range from low values for benzene (4%) to much higher values for pyridine (24 to 50% with a mean of 36%) depending on coal drying (lowers extract yield) and number of steps employed. With CS₂/NMP mostly comparable yields are obtained (20 to 35%, with a mean of 30%) depending on additives. At a higher temperature of 600K a value of 70% has been reported that was attributed to relaxation of the coal structure although a limited bond-breaking would also enhance the yield. Multiple authors have achieved extraction yields in the 60 to 70% range daf basis (HyperCoal related) with a range of solvents at temperatures above 600K although lower values are also present. The chemical evaluations of extract and residue are remarkably similar in bulk properties and NMR structural parameters at low temperatures, the difference becoming more extensive with higher temperature conditions. Upon mixing with the solvent there is a change in enthalpy and entropy of the system and the coal may have the ability to rearrange. Solvents that have a solubility parameter close to Illinois coal will be the most effective. Select ionic liquids have been found to be effective at extensively fragmenting Illinois coal (many particles ~ 10μm being created presumably due to stresses involved at the interface with the solvent front swelling the coal. This offers the potential to enhance coal-catalyst contact in liquefaction and obtain high yields, rapidly or alternative approach to HyperCoal formation.

4. MICROWAVE TECHNIQUES
In collaboration with Drs. Lester and King from Nottingham University (United Kingdom) from the National Center of industrial Microwave Processing, and some of their former and current graduate students, a review of the microwave energy to coal processing was prepared (Appendix A4). The manuscript covers a wide variety of processes ranging from coal drying (or upgrading), liberation of minerals, pre-treatment to improve grindability, liquefaction enhancements, and carbonization into materials such as coke. There is also consideration of analytical techniques that use microwave energy for continuous monitoring of coal feed systems. Where possible, industrial or pilot scale examples of these processes are discussed, along with a consideration of the significant hurdles that exist scaling from bench or pilot scale systems to industrial sized units. As operational scale increases, the frequency of the microwave generator decreases and this is where a rigorous understanding of the dielectric properties of the material and extensive electromagnetic modeling of the applicator is critical. Of particular interest to Illinois coal is the improved removal of pyrite, rapid drying, improved pulverization, and alternative coking processes with the application of microwave energy.

5. MOLECULAR MODELING APPROACHES AND ADVANCES
This report was combined with the major advances in coal science report (see section 8).
6. COKING REACTIONS AND PROCEDURES
With the aid of coal petrologist Gareth Mitchell (Penn State) who did the bulk of the report, the extensive early work on Illinois cokemaking by the Illinois Geologic Survey was reviewed along with the history and transitions in the ironmaking process that has necessitated the curtailed use of Illinois coals except in limited blending roles. There are significant challenges associated with the use of Illinois coals in modern blast furnaces. They can be summarized by challenges associated with 1) their high sulfur content, 2) limited coke strength, 3) high reactivity, 4) moisture content, etc. These are a direct result of the rank, chemical structure, maceral composition, and the thermoplastic behavior of these coals. While Illinois coals can play a limited role in coal blending for cokemaking, future research opportunities with enhanced cleaning (physical and chemical), manipulation of the thermoplastic properties, through treatments such as microwave heating, may enhance their usability and expand their utilization. The full report is in Appendix A5.

7. MACERALS AND HETEROGENEITY
In collaboration with John C. Crelling of Southern Illinois State University, Appendix A6 explores the literature of macerals and heterogeneity with a focus on Illinois coals. Under the microscope the beauty and complexity of coal is revealed indicating the contributions of organic inputs and depositional environments. Macerals contribute to the complexity of coal and the extreme variations in behavior even between similar coals. They are distinguished (reflectance mode) by their differences in reflectance, size, shape, fluorescence, and by color in thin sections. Their structural differences impart density, and hydrophobicity differences that enable effective separation of the maceral groups and separation of density fractions within groups. Unfortunately, obtaining high purity maceral concentrates requires extensive comminution and demineralization thus it is not an industrially viable option. However, there are lithotype differences in benches allowing selective mining, and partitioning of macerals during handling, processing, and comminution this allowing some natural enhancements that can be utilized to further optimize coal utilization. Here the variations between the macerals and their behavior for Illinois coals are explored from an extensive literature review.

8. MAJOR ADVANCES IN COAL SCIENCE GENERALLY (ANALYTICAL TECHNIQUES AND SIMULATION) OVER THE LAST 20 YEARS
In collaboration with Drs. Randal Winans (Argonne National Laboratory), Ryan P. Rodgers (Florida State University), and Atul Sharma (National Institute of Advanced Industrial Science and Technology, Japan) the advances in coal science were explored. The full report is in Appendix A7. There are periodic publications that address advances in coal science. This continues that tradition and focuses on the author’s views of the more significant advances in analytic techniques (chemical and physical) and molecular based simulation that has expanded our ability to quantify coal properties and explores its behavior. During the last two decades (plus a few years) the rationalization of coal chemistry has been considerably expanded by: the additional quantification of solid state $^{13}$C NMR, the quantification of the lattice fringe views from coal HRTEM micrographs, evaluation of molecular weight distribution by laser desorption ionization (LDI) mass spectroscopy (MS), and the inclusion of structural diversity via the Fourier transform ion
cyclotron resonance (FT-ICR) MS approach for coal extracts. Specifically, the Solum et al. combined dipolar dephasing coupled with CP MAS NMR to produce 12 carbon structural parameters was a significant advance in enhancing comparison of coals structural features. With lattice fringe extraction techniques coal HRTEM micrographs went form a hazy micrograph to the elucidation of the distribution of the aromatic lattice fringes, their size, orientation, and clustering across the rank range in coal products. Laser desorption ionization mass spectroscopy has yielded further insights into the molecular weight distributions of coal. Electrospray ionization (ESI) FT-ICR MS is expanding our understanding a coals’ compositional and structural diversity by directly determining the elemental compositions of the ions of coal extracts (by accurate mass measurement alone) and capturing/visualizing the high resolution MS data with Kendrick mass defect plots vs. nominal Kendrick mass plots, heteroatom class consideration, color isoabundance plots, and van Krevelen diagrams.

Physical properties and coal behavior are also further quantified by HRTEM lattice fringe images, porosity evaluation through small angle X-ray (or neutron) scattering (SAXS/SANS) approaches, and X-ray computed tomography evaluations. Specifically the HRTEM lattice fringes shows the distribution of the stacking and orientation of aromatic fringes aiding quantification of aromatic arrangements on the atomic scale. Through SAXS and SANS, particularly at U.S. National lab user facilities, with contrast matching approaches the behavior of coal with gases and solvents has been elucidated. For example the pore filling of CO$_2$ in sequestration related studies has been captured as has changes to the pore structure with in-situ devolatilization or gasification. X-ray computed tomography has allowed the non-destructive evaluation of the physical structure of coal with resolutions in the 35μm range with the promise of significantly higher resolution. This has permitted 3D evaluations of: the cleat structure, quantification of coal swelling/contraction with addition/removal of gases and solvents, determination and anisotropy of strains, kinetics of gas uptake, coking transitions, and impacts of microwave exposure on the cleat network.

Analytical advances have resulted in the ability to quantify coal data and further constrain molecular representations. Restricting models to capturing the average NMR parameters, while capturing a portion of the structural diversity has resulted in new computer aided tools for structure creation and evaluation. Several tools have evolved such as SIGNATURE (Stochastic generation), computer aided molecular design, with advances in the evaluation of the resulting structure (POR-pore size distribution), NMR evaluations, pair distribution modeling, etc. Building on these approaches the state-of-the-art couples HRTEM analysis (diversity of fringe lengths and orientations) to directly construct constrained molecular representations (Fringe3D) which can be manipulated in 3D structures further constrained by: multiple NMR parameters, FT-ICR data (diversity of heteroatom classes for example), SAXS and SANS data for pore size distributions (limited to a limited extent by the scale of the representation). Automated approaches have expanded the scale of representation with greater accuracy and improved ease with improvements in communication of structural information via 3D and 2D lattice structures. Thus, there has been increased utility and applicability for molecular modeling and analytical advanced to the rationalization of coal science.
9. DETERMINATION OF ACTIVE CENTERS OF COAL RESEARCH DOMESTICALLY AND INTERNATIONALLY

This report was written with the contribution of multiple authors and separately addressed the U.S academic institutions in a journal article (Appendix A8a) and country specific discussions in conference proceedings (Appendix A8b-c). There has been a remarkable rise and fall in the frequency of coal science related journal publications from U.S. entities. There has been a passing of the mantle from the U.S. to China as the leading nation for English-language coal journal articles. An ISI Web of Knowledge (using the Web of Science database) evaluation of journal articles with “coal” in the title (in English-language journals) for the periods 1970 to 2010 and 2000 to 2010 was used as an approach to evaluate the historically active and currently active research centers in coal science. This approach underestimates the contributions but provides a basis for unbiased comparisons. Contributions were broken down by research institutions and by countries of contributing authors using analysis tools within ISI Web of Knowledge webpage. The United States has 30% of the publications between 1970 to 2010, with Japan contributing 7.8% and the People’s Republic of China 7.5%. England, Australia, India, Canada, Poland, Spain, Germany, and France contributed between 5 to 2% each. However, China has been the leading country for coal title publications since 2006. The peak publication year for the U.S. was the early 1980s. A decline in U.S. funding opportunities in basic research resulted in multiple once-active coal research centers to focus their efforts elsewhere. This paper focuses on the academic contributions to coal research in the United States and identifies centers that are still active and their focus areas.

The leading academic institutions publication records were evaluated using Wordle to visually determine research focus areas through word frequency analysis of the journal article titles. The Wordle analysis and scanning of article titles determined areas of specialty for the various universities and other institutions. Active authors (for the period of analyses) were also determined using this approach. Among the U.S. academic entities, the leading institutions (by quantity of journal articles) were The Pennsylvania State University (Penn State), Kentucky, West Virginia, Southern Illinois at Carbondale, University of Illinois, MIT, Utah, Brigham Young, Pittsburgh, Ohio State, Virginia Tech, Wyoming, Auburn, Carnegie Mellon, North Dakota, Iowa, California at Berkeley, Tennessee, Texas, Purdue, Texas A&M, Missouri, Georgia, and Western Kentucky. Of these, about half are still “active” in “coal science” as defined as 15 coal science publications (by this search approach) between 2000 to 2010, where the focus is science and engineering research on coal, but does not include coal-related areas such a post-combustion pollution control or the various catalytic interaction of coal synthesis gas.

This work was published as (Appendix A8a):
(Appendix A8b-c):
10. EVALUATION OF AVAILABLE JAPANESE/CHINESE LANGUAGE LITERATURE

It was evident early that there were limited journal publications on coal science in the Japanese language with their contributions being copious in the English language. Thus the focus moved to an investigation into Chinese language(s) publications and was expanded to also consider contributions in the English language publications. Appendix A9 contains the report written in collaboration with Drs. C. Song (Penn State) and R. Finkelman (University of Texas at Dallas). China is now the leading nation for coal in the title journal articles, overtaking the US. There has been a rapid rise in coal research within China as it “fuels” much of the electricity generation expansion but also a coal-to-liquids and coal-to-chemical industry. Research was performed to identify journals active coal science research in the Chinese language(s) and to identify the leading journals and institutions (academic and companies) publishing coal research between 2000 and June of 2012. Unfortunately, locating Chinese language publications, related to coal science, was challenging due to very limited navigation in English and lack of citation collection automation approaches common for English language journals. It was common however to also include English titles and often abstracts too. Furthermore some of the journals were also available in English-language translations indicating a greater desire for an international presence in coal science. Leading journals for quantity of relevant publications were the Journal of Fuel Technology, Journal of China Coal Society its associated Journal of Coal Science and Engineering, with other examples such as: Boiler Technology, Journal of Engineering Thermophysics, Coal Conversion, etc. Thus it appears that there are limited coal science publications in the Chinese language with the greater volume being in English publications.

Articles containing “coal” in the title were identified using the ISI Web of Knowledge selecting only the Web of Science (Science Citation Index Expanded) database for English language publications to identify the leading institutions (2000 to 2012 June). Those with > 100 papers during this period were The Chinese Academy of Sciences, China University of Mining Technology, Huazhong University of Science and Technology, and Tsinghua University. Wordle word cloud plots were produces for these and the other leading 10 institutions to identify regional interests and specialties. There was great interest in coal combustion for many of these institutions, often being the leading subject. In other universities there were obvious specializations in coal gasification, coal liquefaction, oxy-combustion, pollution control etc. Of the journal articles some 29% are published in the journals Energy and Fuels (238 papers), Fuel (204), Fuel Processing Technology (121), and the International Journal of Coal Geology...
This is slightly less than the 33% publications from US sources. The remaining 1653 articles from China are incredibly well dispersed among 404 other journals with only eight of those journals having more than 30 articles. The other US articles were similarly well dispersed (469 journals). Clearly Chinese coal science has a significant number of coal publications in the leading coal science journals. The greatest frequency of collaboration (up to 25% of the papers) was between the U.S., Australia, Japan, and England (Appendix A9).

11. HOW CAN THE STRUCTURE BE USED TO PRODUCE PRODUCTS OTHER THAN LIQUID FUELS OR ENERGY APPLICATIONS?

An earlier ICCI project (10/7B-3) supported the creation of a large-scale atomistic representation of Illinois no. 6 coal. This structure contains 50,789 atoms within 728 molecules and is the largest, most complex coal representation constructed to-date. It was based on an extensive review of the available chemical and physical structural data for this Argonne Premium Coal. Specifically the aromatic ring size distribution was based on multiple HRTEM lattice fringe micrographs. These were duplicated with automated construction protocols (Fringe3D) in molecular modeling space and cross-linked to accommodate both molecular weight distribution data and NMR parameters. Similarly the distribution of functional groups was captured based on an array of published data. Given the large-scale and improved capture of the molecular diversity can the structure have utility in the optimization of strategies for the production of specialty chemicals and feedstock? The oxidative hydrolysis dissolution of coal (OHD process) developed at SIU Carbondale, is one such approach for the production of these desirable products.

Advances in simplifying the chemical complexity has been achieved through atomic typing from molecular modeling force fields and graph theory to identify and collapse benzene/PAH/hydroaromatic ring structures and cross-links into nodes and linkage line producing a 3D and 2D lattice structure. The 2D lattice is reminiscent of Bethe lattice structures except here it is specific to a particular molecular representation of coal. Using these lattice structures allows the communication of structural information of the full-scale model through color manipulation of the nodes and linkage lines. Similarly the molecules (single nodes to multiple nodes connected by linkage lines) can be similarly manipulated to show relative position, solubility estimates etc. The greatest potential however comes from kinetic modeling of the thermolysis process, albeit in a simplified process, based on the kinetics of benzene-cross-link-benzene kinetics. This allows consideration of the thermal breakup of the network structure. Thus we have the ability to perform relatively rapid initial simulations that can aid in selection of conditions for specific production of molecules. While there is more work to do in progressing this approach it shows how an intimate knowledge of structure can be utilized for the improved rationalization of coal. Improvements in mass transfer consideration, gas formation, cross-link and thus kinetic complexity, addition of retrogressive reactions, and demonstration of the capability with simulation being tested against experimental results will be the true test of this advancement (Appendix A10).
12. RECOMMENDATIONS FOR ILLINOIS COAL

We are in an era of funding challenges for the progression of basic and applied coal science during while the coal industry continues to face challenging times and considerable uncertainty. For the effective leveraging of Illinois Clean Coal Institute (ICCI) funding should be highly directed, serve the current and future needs of Illinois coal producers and Illinois-coal users. Thus, the institute needs to return to its roots both for new knowledge creation and ensuring a skilled workforce is in place to tackle issues of relevance to the Illinois coal extraction and users. This entails soliciting, encouraging and funding of “hands-on” coal research, especially at Illinois-based institutions. Specifically:

12.1 ENCOURAGE “FREE” ILLINOIS COAL RESEARCH

One of the most effective uses of funding is to support activities that promote Illinois coal research – with funding from other sources. This includes federal funding opportunities in coal research that should be widely disseminated to Illinois researchers to encourage entry into coal research and to better ensure continuation of currently active centers and institutes. It is desirable to take stock of the academic talent pool (targeting specific strengths) in Illinois and encourage entry into the coal science field.

The incorporation of Illinois no. 6 coal in the Argonne Premium Coal Suite\(^1\) has resulted in copious “free” research for Illinois. It is the most well studied coal in existence.\(^2\) The continuation of the Argonne Premium Coal Program and wider dissemination of Illinois no. 6 data will promote additional research utilizing this coal standard. Dissemination of the journal publications (and encouragement of ICCI funded work to result in journal articles) will aid its continued use. A modern web-based (searchable by topic and coal) Argonne Premium Coal database will further promote the use of Illinois no. 6 coal in research both domestically and internationally. An earlier ICCI funded program resulted in three publications of note, one being an extensive review of the available data,\(^3\) the creation of a state-of-the-art downloadable large-scale (50,000 atoms) atomistic representation,\(^4\) and an example of the oxidation and combustion of an Illinois coal char.\(^5\) It is expected that the review and the coal model will aid in encouraging use of this structure enhancing the leverage from its original investment.

12.2 INCREASE ILLINOIS HUMAN CAPACITY

As indicated earlier there should be efforts to increase awareness of federal and other funding opportunities to Illinois academics. There should be a seeking out of those working in related fields and expose them to coal research opportunities to aid increasing both coal knowledge but also increased human capital. Illinois coal researchers and others should seek active partnerships with other coal-research universities. Domestically, the most active are Penn State, West Virginia, and Kentucky. A fuller listing with identification of U.S. institutional specialty is available.\(^6\) Research centers in the UK, Australia, and South Africa have also been identified,\(^7\) as have Chinese institutions (currently the leading nation for the publication of “coal” English language peer-reviewed journal articles-see earlier sections of this report). The future of coal science will have to be more collaborative given the changing nature of the research and the retirement of the talent pool put a strain on our capacity. This can be encouraged with
travel funding for students/researchers for training and collaborative research. Likewise collaborative research and development should be encouraged. It is essential that those currently active coal centers in Illinois remain active. Loss of these entities will likely be permanent or very cost prohibitive once inactive.

It is recommended against funding coal-related areas that are well funded by federal funds. Leveraging ICCI money though cost-share in federal funding has a high return on investment, funding fields that have support such as basic FT catalyst development has a lower return on investment (some Illinois-specific challenges such as higher sulfur content would be reason to continue funding). Thus, unless strategic for personnel retention, Illinois-specific challenge related, or to encourage entry into a field these funds are likely to have a more significant impact elsewhere. Direct coal research such as coalbed methane or CO₂ sequestration etc. should still be supported even if there is ample federal funding as it aids to Illinois coals industry readiness and human capacity building.

12.3 EXPLORE OPPORTUNITIES IN COAL PROCESSING FOR EFFICIENCY
GAINS
In an era with the possibility of greenhouse gas emission constraints or emission taxation the economics of coal preparation (including beneficiation/cleaning) will change and efficiency gains become more important and should be re-evaluated. Coal drying is one such opportunity as it enhances the calorific value, improves pulverization efficiency, reduces water usage, and reduces emissions. Microwave applications coupled with waste heat could be one approach that also has the potential to aid mineral matter rejection in the coal cleaning process (see microwave report earlier in the appendix). Select ionic liquids have also shown the capacity to fragment Illinois coal extensively and may offer improvements in HyperCoal creation, direct coal liquefaction, and mineral matter rejection. The recycling of the ionic liquid is an important aspect (see report on solvent swelling and extraction earlier in this appendix). Combinations of coal preparation, drying, and novel treatments may have synergies and produce even better returns. Thus, a return to coal mineral processing research is warranted to better prepare for potential impacts from greenhouse gas management legislation.

12.4 COAL-TO-LIQUIDS
As the report, earlier in this appendix, indicated there are ample opportunities for an Illinois-based coal-to-liquids industry. The high sulfur content and pyrite (iron) aid the direct liquefaction process and Fe also aids gasification reactivity of coal chars. Exploration of the use of direct liquefaction resids would be helpful either for specialty carbon production or fuel use. Continued support for hands-on coal direct- and indirect-liquefaction (gasification) is appropriate. Also the incorporation of an Illinois appropriate biomass co-feed would likely be of aid for emissions and economics. Mineral processing advances may produce more appropriate cuts of coal as discussed in the maceral heterogeneity report earlier in the appendix. The oxidative hydrolysis dissolution of coal is a very promising advance and should continue to be supported. Specific interests should include scale-up, product analysis and separation, also exploration of use of the feedstock such as specialty polymers, etc.
12.5 USE OF COAL SCIENCE IN THE PROCESSING AND USE OF COAL
Promote advances in the use of molecular structure, kinetic data, and molecular modeling for optimization and exploration rather than informed trial and error commonly employed. Advances in analytical techniques and in molecular modeling approaches are discussed earlier in the appendix.

CONCLUSIONS AND RECOMMENDATIONS

Specifically I was asked to provide recommendations for a 5-year and 10-year time frame. However, these recommendations span both of the time frames. Recommendation 1 has the highest priority because of its low cost (with the exception of the cost-share on federal funded projects). Human capacity building remains an important challenge and is accommodated by continued support in all of these areas suggested but particularly in recommendation 2. Continued progression in coal-to-liquids is durable with OHD as a strategic high priority given its initial success with continuation of coal-to-liquids interest expected over the next 10-years (recommendation 4). It is suggested that recommendation 3 be adopted within the next few years with ramp-up over the decade. Its impact depends on the timing of legislation and a willingness to reduce greenhouse gases (including incurring the added expense). It is desirable to be well ahead of this curve so the priority should be adjusted depending on the external influences. Of all the recommendations the use of Coal Science in the Processing and Use of Coal already occurs but its expansion requires advances in both analytical techniques and simulations. Considerable success has been achieved in this area and the adoption of advanced analytical techniques should be encouraged. The use of molecular models will be a harder sell and should only be extensively promoted when there has been a demonstrated ability. It is already helpful in exploring structural transformations but progression is needed before it is a standard tool in the coal scientist’s toolkit.
REFERENCES

DISCLAIMER STATEMENT

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