BLG
Black Liquor Gasification

Assessment by the Scientific Review Panel

17-19 May, 2006

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A. Introduction

The assessment focuses on the scientific quality of the programme seen in an international context and includes comments on the overall relevance. The members of the review panel are listed in Appendix 1.

The assessment is based on the Progress Report from the BLG Program 2004 – 2006 including a list of publications and the BLG II Program Proposal for 2007 – 2009. The review panel met with the applicants on May 18 (9.15am – 1.30pm) and had the opportunity to ask questions to clarify the thinking behind the programme. The participants in the hearing are listed in Appendix 2.

B. Conclusions and Recommendations

- Sweden is a world leader in the production of high quality pulp and paper products and in supplying processing technology options to the world market. The high temperature black liquor gasification technology being developed by Chemrec has both scale up and process efficiencies that are superior to competing technologies.
- The key patents on the technology are Swedish, which means that a large scale commercialization will create business opportunities for the Swedish industry also outside of the pulping industry.
- Successful implementation of the technology in Sweden can have a major impact on the electricity production or, alternatively, an even greater impact on renewable fuel production for the transportation sector.
- The research programme interacts with and supports the process development project connected to the demonstration plant (DP-1). This secures strong contacts between academics and industry.
- At the end of Phase I most of the program goals and deliverables will have been met. The Panel judges the scientific quality and publication rate as good/very good. The BLG program team has responded favourably to the suggestions made at the May 2004 program review. Sub project leaders have clear responsibilities and the program director has created a cooperative team environment.
- The Panel finds the Phase II program is well designed and well structured to take advantage of the unique DP-1 facility in Pitea, which represents a huge prior investment of time, money, and expertise. If the goals of MISTRA program are met, this will make a significant contribution to enabling the near-term commercial deployment of BLG technology.
- The review panel is of the opinion that MISTRA should fund the programme proposed in the document *The BLG Program: Black liquor gasification – enabling technology for renewable transportation fuels* for 2007 – 2009 with due consideration given to the recommendations in this report.

C. Review of Phase I Sub-Projects in the 2004-2006 BLG Program

Sub-project 0: Synthesis of Results and Project Coordination
Project Leader: Rikard Gebart, ETC

Relevance
Synthesis of results, project coordination and team leadership is a pivotal role to ensure project success. The MISTRA panel program review of May 2004 expressed some concern that the program as presented then was very complex in structure, was in need of more clarification of group responsibilities, should consider outreach to more international cooperation and should make sure that the program director dedicated sufficient time to ensure effective program leadership. These things were felt to be very important to the success of the BLG Program.

Scientific Quality and Results
The review carried out on May 18, 2006 clearly indicated that the BLG Program team had responded favorably to all of the above the above suggestions. Sub project leaders were identified with clear responsibilities. A Scientific Advisory group consisting of world class scientists from Sweden, Finland and the United States has been formed and meets at least twice per year. These meetings are held in conjunction with IEA Annex 15 meetings, effecting a productive outreach and exchange with a large group of researchers working in relevant areas. Effective cooperation has been established with a number of laboratories in Finland and the United States. It also appears that the Program Director is effectively managing his time commitment to the program and has created a cooperative and productive team environment. The May 2006 Scientific review panel was impressed with the results in the project coordination area.

Sub-project 1: Modelling, Simulation and Optimization of a Downflow Entrained-flow Reactor for Pressurized Black Liquor Gasification
Project Leader: Rikard Gebart, ETC

Relevance
The objectives of this subproject were to 1) develop a computational fluid dynamic (CFD) model of the high-temperature reactor section (burner and primary reaction vessel) of the pressurized, oxygen-blown Chemrec black liquor gasifier (BLG) design to aid in design of future demonstration and commercial-scale units; 2) perform spray characterizations of the burner nozzles to aid in the CFD modelling and reactor design optimization, and 3) to obtain experimental data to validate the modelling work.

Being able to predict the multi-phase flow and chemistry in the high-temperature sections of the BLG is critical to being able to successfully scale up the design for commercial applications. There is little-to-no prior fundamental scientific understanding of how to predict the interacting multi-phase fluid flow, chemical reaction, and heat transfer that occurs in the hot section of a BLG. This sub-project built a CFD modelling framework that incorporates fundamental scientific understanding (developed in this and other sub-projects) to predict reacting flow characteristics.

Scientific quality and results

The sub-project to date has 1) built a pressurized nozzle (cold) spray test facility and carried out some testing (using water/syrup mixtures) of alternative nozzle designs, 2) developed a self-consistent comprehensive CFD model of the hot reactor sections (implemented in a commercial CFD software called CFX), and 3) carried out some initial model validation using preliminary data from the DP-1 pilot plant facility. The model is for a ceramic-lined (~adiabatic) reactor design. (Originally planned work on modelling of a cooled-wall reactor was not pursued, since Chemrec has determined that this design is unlikely to be commercially viable.) Building on prior licentiate thesis work (by Marklund), a strong model framework has been built. Several articles on different aspects of the model have been published, including one in a top peer-reviewed scientific journal (*Combustion Science and Technology*), attesting to the high quality of the model development work.

The model has not yet been fully validated with experimental results (due to lack of experimental data thus far). Also, there is fundamental scientific work ongoing (in other sub-projects), the output from which remains to be incorporated into the model before the completion of Phase I of the overall project. A key focus of the remaining current project and in the proposed Phase II project is to data collection and model validation.

Sub-project 2: Modelling of the Quench and Counter-Current Condenser
Project Leader: Lars Westerlund, Lulea University of Technology

Relevance

The objectives of this subproject were 1) to develop a CFD model for the quench and for the counter-current condenser for use as design tools for future scale-up and 2) to use measurements from the DP-1 pilot plant to validate the models.

The quench stage of the BLG process cools the raw syngas rapidly from about 1000°C to about 220°C by spraying condensate onto the gas and smelt mixture leaving the hot reaction section. The heavier smelt particles fall into a water bath (forming green liquor) while the cooled gas and smaller entrained smelt particles travel to a separate condenser stage, where they are further cooled (condensing out liquid) by passing over tubes inside which low-pressure steam is raised. The condensate is used as the quench fluid. Accurate models of the quench and condenser units, including ability to predict green liquor quality, would be important aids for designing commercial-scale units. No such models are currently available. In the case of condensation, techniques for using condensation are well-understood for many applications, but an accurate CFD model would enable inexpensive exploration of alternative geometries and designs to optimize the performance and minimize cost for this major piece of equipment in a BLG system.

Scientific quality and results

A simplified model of the quench (implemented using a commercial CFD code, FLUENT 6) has been developed during the sub-project. The model has been exercised to predict flow rate and temperature distributions in the quench under different assumed operating conditions. There has not yet been any validation of the quench model with data from the DP-1 plant, but preliminary comparisons with performance expected by the designers of the DP-1 quench show inconsistencies. These may be due to the simplifications used in constructing the model, including leaving out chemical reactions and excluding the film flow section of the quench vessel. The latter simplification may not be as important as the former. Adding chemical reactions into the quench model is expected to improve the accuracy of the model (and is especially important for predicting green liquor quality) and doing so is planned as part of the final efforts in Phase I of the overall project.

The incomplete work on the quench model is due in part to the larger-than expected effort required to develop the CFD model of the condenser. The condenser model has been constructed, but the overall performance it predicts does not compare well with overall expected performance (from the designer's calculations) of the DP-1 condenser.

Further work is needed in the development of both the quench and condenser models, and validation using DP-1 data is also needed. Because of the incompleteness of the modelling effort to date, results have not yet been published in the peer-reviewed scientific literature. Such publication would help validate the quality of the work being done.

Sub-project 3: HT BLG Inorganic Process Chemistry - effects on gas phase, smelt, particles, container materials and green liquor quality

Project Leader: Anders Nordin, ETPC, Umeå University

Relevance

Black liquor, being a high "ash" fuel and the source of inorganic cooking chemicals in the closed loop of the pulp mill, reacts in HT BLG very much depending on the inorganics. Their behavior in the process controls the melting point, the catalytic gasification, the distribution of sulfur between Na2S and H2S (it means the distribution between the gas and the melt/green liquor), and also affects the ceramic containment material.

Reliable and accurate fundamental thermo chemical data for use in understanding and modelling the controlling reactions are thus of utmost importance.

Scientific quality and results

The ETPC group has excellent background for these types of studies and the group has been strengthened with several senior researchers in the field in parallel with younger PhD's and PhD students.

Initial literature review indicated major inaccuracies in some of the most important data such as distribution of sulfur.

Equilibrium models based on available literature data and statistical experimental planning models were used to estimate the influence of the inaccuracies in input data to the results in the theoretical model. That was the basis to select a few reactions that needed new experimental studies to narrow the possible theoretical variations. Beside the results from the work a model "Sensitivity analysis" was developed.

The group adjusted the program to more thermodynamic data and less effort to produce kinetic data after advice from the scientific council May/June 2005.

Several advanced testing methods have been used such as High Temperature Microscopy (HTM), Thermal Analysis/Differential Scanning Calorimetry (TA/DSC) and High Temperature X-Ray Diffraction (HT-XRD) to generate and confirm data.

The project-generated data and literature data have been fed into the other subprojects such as CFD-modelling in task 1 and 2 together with a four box simplified reaction model.

DP-1 sampling methods and sampling probes have been suggested and will play an important role once the closer validation of the reactor modelling works starts (mainly in next project phase).

The new experimental studies partially with new technology such as EMF have been able to narrow the theoretical uncertainties in the sulfur distribution from 68+/- 16% to 70 +/- 2 % as H2S in gas. These results as well as the sensitivity model are published in Journals like Energy and Fuels and J. of Chem. Thermodynamics and others. Several contributions to conferences and other meetings have been presented as wells as PhD thesis.
Further data on COS, CS_2, S_2 new data NaOH (g) and several phase diagrams will be produced and published within this project period.

Sub-project 4: The kinetics of the gasification of black liquor
Project leader: Tobias Richards, Chalmers University of Technology

Relevance
The general behavior of black liquor in gasification processes is studied over the years including the main steps – drying, devolatilization/pyrolysis and gasification/melting.
For the HT BLG- process there is a need for specific kinetic data relevant for the chosen operational conditions in the process: small droplets (< 100 micron) in entrained flow at high pressure 3 MPa and high temperature 950- 1000 degree C.
Extrapolation from one set of data at other conditions to the actual DP-1 conditions is not possible because the limiting reaction step will be different and the information necessary is not included in the data from another operational regime.
Accurate kinetic data is of major importance for the modelling and interpretation of DP-1 results.

Scientific quality and results
The initial approach at CTH was controlled by the equipment available and the possible experimental parameters in that equipment. That meant studies in a thermo balance of 3-5 mm particles including swelling and later droplet description through mathematical modelling
After advice from scientific council changes from original plan took place:

- Less focus on droplet model
- Kinetic expression from powder material
- Pressurized experiments (pyrolysis and gasification condition) at IPST

Further testing is planned at IPST. The existing equipment at IPST can only use dried black liquor.

Droplet gasification results for 3-5mm particles have been presented including swelling for different types of black liquor. A reasonable mathematical model for that particle is developed. Test with an atmospheric drop tube furnace LEFR for small particles have been performed. The swelling behavior and particle modelling have been presented at conferences and in two master thesis.
The result from CTH seems not to be directly applicable to the modelling for the DP-1.The results from IPST will probably be more applicable but it is hard to judge as they have not been presented yet.

Sub-project 5: BLG with Borate Autocausticizing
Project leader: Ingrid Nohlgren, ETC

Relevance

Positive results of adding borate to conventional recovery systems to decrease the load on causticizing created some degree of excitement concerning the impact a similar approach might have in a BLG recovery cycle. This excitement was fueled by the need to find a solution to the increased causticizing load that results from the BLG technology. Sub Project 5 was organized to pursue this possibility.

Scientific Quality and Results

The Scientific Review Team believes that the project was organized and executed very effectively. The project leader developed an experimental approach to achieve a convincing laboratory demonstration of the borate autocausticizing effectiveness with BLG. This was a good example of utilizing international cooperation as the most cost effective way to achieve the result. The work was carried out at the Institute of Paper Science and Technology at Georgia Tech.

The results were convincing. Borate autocaucticizing as applied to BLG was found to be not effective. This result was disappointing and counter to what was expected. However, it is an important result because it forces other directions to be taken to solve the increased load problem present when BLG is utilized in the recovery cycle.

Sub-project 6: Pulp Produced from Liquors Utilizing New Recovery Systems
Project leader: Leelo Olm, STFI

Relevance

The separation of sulfur and sodium made possible by application of the BLG recovery technology opens the door for new and improved approaches to pulping . One such process is referred to as the ZAP (Zero Alkali Pretreatment) process. Taking advantage of the sulfur – sodium separation is quite important to the overall economics of utilizing the BLG recovery process. It is believed that pulp yield increases of 3 to 6 percent or more are possible. This will be very attractive to most pulp mills and will be a significant selling factor for installing the new technology.

Scientific Quality and Results

A well designed but limited experimental plan was devised to determine possible yield gains utilizing ZAP pulping compared with conventional kraft pulping and to see if the yield gains would be retained through bleaching of the pulp. Well proven techniques were used by competent technicians for the experiments. The analysis was carried out in a competent and understandable way.

The results showed that all BLG-ZAP pulps did attain higher yields than the conventional cooking and that these gains remained through bleaching. These gains attributable to ZAP appear to be in the range of 2% +/- on wood. It was also noted that important pulp properties were not compromised. It was found that slightly more bleaching chemicals were consumed. These results are encouraging. However, there may be other as interesting or even more interesting pulping approaches that take advantage of the BLG enabled split in chemicals and these additional possibilities should be evaluated as the program continues.

Sub-project 7: Chemicals Management in a Kraft Pulp Mill with a Pressurized Black Liquor Gasification System

Project Leader: Niklas Berglin, STFI

Relevance

The overall objective of this sub-project was to develop a better understanding of issues that may arise with management of chemicals at a kraft pulp mill using a BLG in the recovery area. It is well understood that introducing a BLG into the recovery area of a kraft mill will result in the need for different approaches to management of chemical cycles in a mill. For example, purging of non-process elements can no longer be done as it is today – at the electrostatic precipitator on the exhaust stack of the recovery boiler. Demonstrating and understanding in detail the changes in chemicals management that will be needed with introduction of BLG is a prerequisite to implementing a commercial BLG unit. An effective way to develop this understanding is by use of a whole-mill process simulation modelling, as has been done in this sub-project.

Scientific quality and results

The model has been developed to include a simplified representation of the BLG (the predictions of which match well with data available to date from DP-1), as well as detailed representations of all other relevant elements in a kraft pulp mill. The modelling work shows a thorough understanding of the relevant fundamental chemical processes and an extremely effective implementation of the fundamentals into a highly useful tool for design and analysis. Peer-reviewed articles have not yet been published, but based on earlier modelling work by the scientists involved in this sub-project, the scientific quality of the current work is high.

The whole-mill modelling work carried out as part of SP-7 predicts that a mill with BLG will likely require less make-up sodium. It also predicts an increase in potassium and chlorine concentrations of 50-100%. These are original and informative results. A literature study was conducted on alternative options for purging such NPEs. Plans for the remaining months in the Phase I project are to incorporate NPE purge method(s) into the whole-mill model, on the basis of which some economic assessments will be carried out.

The modelling work has been supplemented with some key experimental work to develop solubility data for some compounds under temperature conditions for which data are lacking (since such data have not previously been needed), e.g., for Na_2S, K_2S, and Na_2CO_3 at temperatures between 100°C and 200°C. Modelling using these new data suggests a risk of Na_2CO_3 precipitation in the quench of the DP-1 plant (where there is no such risk at temperatures below 100°C).

Future plans also include assessing potential scaling problems and further validation of models using data (if available) from the DP-1 facility.

Sub-project 8: Material test in green liquor at high temperature

Project leader: Lars Troselius, Swedish Corrosion Institute

Relevance

Stainless steels are susceptible to stress corrosion cracking in hot alkaline solutions and since green liquor in BLG is much hotter (+100 degree C) than green liquor from recovery boilers the goal is to find materials with acceptable life in hot green BLG liquor. This is a prerequisite for commercialization of the BLG-technology and thus very important.

Scientific quality and results
Material testing is more a question of appropriate testing procedures and good selection of material candidates than pure science. The preparation of the testing samples and introduction of the specimens in the quench vessel and the counter current condenser seems very professional. Due to the delays in the operation of DP-1 the accumulated testing time is yet too short but some conclusions are expected to be drawn by the end of the year 2006 if the time on stream can be increased according to expectations to a total of up to 2500 hours. The special test loop for circulation of hot green liquor when the reactor is idle seems to be well designed and some initial problems discovered during safety HAZOP are now solved. Once the loop can be fed with typical BLG green liquor the test can go on rather independent of the DP-1 operation.

Any conclusions must wait for adequate exposure time to make a fair comparison between candidate materials but a successful outcome is reasonable due to the effective experimental design, which includes many (10) candidate materials and total number of samples (156) with different preparation and location.

D. Review of Phase II Work Packages in the proposed 2007-2009 BLG Program

1. Problem to be Addressed

Black liquor gasification is a key technology for enabling more diversified production at chemical pulp mills and an enabling technology for the concept of a Forest Biorefinery which is gaining attention world wide. The spent liquors from Kraft pulping operations—black liquor—contains about half the energy of the wood input to a Kraft pulp mill, along with all of the spent pulping chemicals (Na2S and NaOH) used in the Kraft process. Black liquor is currently burned in Tomlinson recovery boilers to generate steam and recover pulping chemicals for re-use. The steam is expanded through a turbine to make electricity that meets a portion of the process electricity needs. Some steam is extracted from the turbine to provide all of the process steam needs of the mill. The Tomlinson boiler is old technology (>70 years), relatively inefficient, high maintenance and prone to occasional catastrophic smelt-water explosions.

Many of the Tomlinson boilers now operating, particularly in the United States, will reach the end of their 30–40 year lifetimes over the next 10 to 20 years. As a result, there is a great deal of interest in the pulp and paper industry in having improved black liquor processing technology commercially available in the 2010 time frame. At the same time, there are growing public interests in expanding the role of clean renewable energy to address energy security and environmental concerns. These private and public interests can potentially both be met by commercial implementation of black liquor gasification.

Conversion of black liquor into a synthetic gas significantly enhances energy recovery and diversity of chemical/energy products from the black liquor and reduces environmental impact. BLG offers the potential for up to 7–10 percentage points higher thermal efficiency; higher flexibility in preparing pulping chemicals, leading to the opportunity to implement higher-yield pulping strategies; provides options for creating new value streams in the form of electric power, liquid fuels and/or chemicals; significantly lowering the environmental footprint because of reductions in the emission of particulates, SO_2, NOx, HAPS, VOC and TRS and offsets of CO_2 emissions as a result of reduced fossil fuel usage; and significantly improving safety as BLG eliminates the danger of smelt-water explosions.

The development of BLG technology has been underway for several years and the technology that is emerging as most applicable for large scale application world wide is the high temperature, pressurized, oxygen blown technology being developed by Chemrec. However, there remains significant developments in technology and in fundamental understanding to achieve success. The recent success in building and initial operation of a large pilot plant in Pitea, Sweden provides an opportunity for rapid commercialization and deployment. This and the network of universities and researchers that has been assembled to address these challenges creates a very strong and practical research environment unique in the world.

2. Scientific Value

The proposed program is effectively organized into five interacting work packages dealing with 1) gaining the most value from data taken at the Pitea pilot facility DP-1, 2) utilizing this data to understand the chemical and physical nature of processes going on in the reactor, in the quench and in down stream processing, 3) understanding how the BLG recovery cycle can be optimally integrated with a host mill, 4) using this understanding and knowledge gained in work package 5 to develop verified and useable process models and 5) developing a solid understanding of the fundamental chemistry associated with reactions taking place through the BLG system. Through collaborations, with researchers in Finland and the United States as well as participation in IEA meetings and international conference participation, the BLG II Program team has produced a proposal that is relevant and will contribute to current international research. It should be pointed out that this proposed program is unique and is enabled by prior R&D work leading to the present facility and support team at Pitea.

The program in aggregate will make unique scientific contributions not only to the successful commercialization of the gasifier but also to the basic understanding of the physics and chemistry involved in processing spent pulping liquors at high temperature conditions, as well as whole-mill impacts of introducing BLG recovery systems.

If successfully executed, the planned scientific deliverables will significantly advance the BLG technology and its broad application. The Scientific Review Team, however, believes that some of the proposed program elements are of higher priority than others and will comment on this in the report below.

3. Program Structure

As commented on in the review of Phase I above, the Scientific Review Panel believes that the BLG Program team had responded favorably to suggestions made in a prior review. Sub project leaders appear to be tasked with clear responsibilities. The formation of the Scientific Advisory Group is a very positive step. Holding these meetings in conjunction with IEA Annex 15 meetings is an excellent way to effect productive outreach and exchange with a large group of researchers working in relevant areas. Effective cooperation has been established with a number of laboratories in Finland and the United States and it appears that the Program Director is effectively managing his time commitment to the program and has created a cooperative and productive team environment.

The consolidation of the program into five "Work Packages" as described above (rather than the institution-based structure of Phase I) appears to be an effective program structure and reflects the current internal confidence of the team. The management structure has been simplified from Program I and now consists of the five work area leaders reporting through the program director to a steering group that in turn reports to a program council where all sponsors are represented. The Chemrec process verification and development activity also reports to the same steering group allowing for close coordination between the two programs. The Scientific Review Team still finds this structure a bit complex but understands that it is likely necessary to be sure that the many interests are represented. The structure appears to be working smoothly and the Program Director appears to be doing an excellent job.

4. Skills and Networks

The scientists and engineers involved in the program are highly skilled and many have world class reputations in the program areas. Networks and linkages have been dealt with to a large degree above. It should, however, also be pointed out that the link the program team has to the technology owner Chemrec and the Kappa mill in Pitea is quite unique and extremely valuable. There are few mill managers that are forward thinking enough to be willing and able to allow a technology like BLG to be closely linked to the normal operation. The involvement of mill management and operations people is a real plus to this program. The challenges to successful completion of the proposed Phase II work (especially measurements in harsh BLG conditions) should not be underestimated. The review panel heard from the project team of the humility they gained in the course of Phase I work. A similar or greater level of humility in addressing the challenges in Phase II will be needed to ensure success.

5. Component Projects

Work Package 1: Experiments in DP-1

Project leader: Henrik Winnika, ETC

Relevance

The experiments in DP-1 are not only the stepping stone for further scale up of the Chemrec HT BLG process and necessary for the commercialization of the technology but also the final test of most parts of the supporting research program, including the CFD-modelling work and all the sub-models and other small scale testing in the research program. Besides validating the models the test results might raise new more or less fundamental questions to be studied in the support program.

Scientific quality and approach

As long as only inputs and outputs to DP-1 are measured, the reactor is a black box. It is therefore important to start measuring inside the reactor and quench. Due to the difficult (high pressure, high temperature, corrosive) environment including reacting gases, melt and perhaps tar and soot/char the measuring problems are very challenging. Major efforts and possibility in the budget for allocating further efforts to this should be planned for due to possible difficulties.

With all the technical challenges facing the tests for process verification and further commercialization it is still very important to put a priority on the sampling, measuring and testing to verify and give feedback to the research program. The allocation of some of the operational costs of DP-1 to the research program is relevant and justified.
Comments to some of the subtasks:
ST1.1.3: The application of new sampling methods is of major importance and includes the difficult task to sample smelt and solids.
ST1.1.4 Considering the corrosive environment especially the in-situ oxygen measurement with lambda sond seem to be very difficult.
ST1.1.5 and ST1.4 "Tar" definition, sampling and measurement have been a major issue in the biomass gasification community for many years to achieve reliable data. An EU-Project "Tar Protocol" has developed standard procedures that have been tested by different laboratories. Swedish contact points have been TPS and RIT. Advice on current methods should be taken before developing " new" methods.

ST 1.2.1 and ST 1.4 Before starting a new "fundamental " tar formation and conversion program (WP 5:1) it is important to measure the overall results in DP-1 . See further comments on this under WP 5. If the measurement confirms the results from early tests in Karlstad the situation is simplified and the effort can be focused on how to handle the minor PIG compounds in process train rather than to explain all the details of formation and destruction.
ST1.2.2 Gas sampling and characteristics are of great importance but also needs to be carefully analyzed to assure that the results reflect the situation in the reactor rather than secondary reactions in the sampling train on the solids or in the condensed liquid phase.
ST 12.3 The alkali distribution in gas and on solids such as soot, char is very interesting but again a challenging task to actually reflect the situation in the reactor after sampling.
ST 1.3.1 The smelt sampling is again a very difficult task. The other sampling points suggested are more inline with conventional technology.
St 1.5. Material testing and evaluation are still a task of major importance in the next project phase.
Besides being crucial for the further development of the process, and validating the earlier research, the experimental testing will yield valuable testing methods and new sampling techniques that can be applied to other processes.
The DP-1 testing is **the number one priority** in the development of the BLG technology. Every possible effort should be taken to achieve steady state and long-term operation of the DP-1 test plant even if some other parts of the program have to be reduced in scope.

Work Package 2: Applied Process Chemistry

Project Leader: Rainer Backman, Umea University

Relevance
Work package 1 will develop leading edge techniques for sampling gases, particulate, smelt, oxygen and organic components in the hostile environment of the reactor and quench vessels and at operating pressure of up to 30 bar and temperatures of up to 1000 degrees centigrade. Most of these measurements have never been achieved before in this environment and will require innovative new methods. The need to do this, however, is compelling and represents one of the major reasons for constructing the pilot plant. Work package 2 will utilize these measurements and droplet formation studies to develop understanding of the complicated chemical and physical nature of pressurized BLG processes and use this understanding to help

develop and to verify process models. Without completing work package 2 the value of work package 1 is minimized. Work package 2 is divided into four overall objectives dealing with: 2.1) analysis and interpretation of work package 1 to increase understanding and help define further data needs, 2.2) creating reliable models for smelt flow and its effect on performance, containment materials and carbon conversion, 2.3) developing aqueous solution models that will estimate solubilities at high green liquor temperatures and 4) create a useable model to describe particle (carbon?) separation in the countercurrent condenser.

Scientific Quality and Approach

2.1) Using the Output of Work Package 1

The value here is extremely high since understanding the physical and chemical phenomena inside the reactor has high scientific value and is key to successful operation and model development. A concern here is that the program plan calls for carrying out the analysis on only one operating condition. If problems occur with that condition and/or with one or more of the sampling techniques in work package 1 this may be inadequate. This task is seen as a very high priority and should be reviewed to see if the plan is adequate.

2.2) Creating Reliable Models for Smelt Flow and Its Impact (Hot Reactor Products)

The value here is also extremely high for the same reasons as stated above. The plan here appears quite robust and should be adequate. The deliverables are well described.

2.3) Developing Aqueous Solution Models

As presented the value of this task is not clear nor is it clear that the approach will yield the desired results. The focus seems to be more on developing an experimental approach and running tests. The leap to how this will effectively result in useful CFD and applied solution models is not explained and needs to be carefully reviewed before proceeding with this task.

2.4) Useable Model to Describe Particle Separation

The value here, as presented, is questionable. The goal of having a CFD model to help optimize the quench and countercurrent condenser is understandable. However, from the information presented the Scientific Review Panel is not convinced that the goal will be achieved.

Work Package 3: Mill Integration and Systems Analysis

Project Leader: Niklas Berglin, STFI

Relevance

WP-3 has two fairly distinct sets of activities, one focusing on non-BLG aspects of a pulp mill that incorporates BLG and one that focuses on some BLG-specific aspects.

The non-BLG aspects will focus on helping to provide an understanding of potential impacts on and opportunities for non-BLG processes at a kraft pulp mill (or pulp and paper mill) when BLG is introduced. Without such understanding, mill owners will be reluctant to invest in commercial BLG systems. This aspect of the proposed WP-3 effort will also potentially deliver useful understanding on which government policy makers might make better informed decisions about incentives that might be provided to encourage BLG adoption. In these respects, these aspects of WP-3 are not directed toward assisting in the development of the BLG technology *perse*, but rather toward essential work needed before the technology is likely to be adopted commercially at any mill. This is clearly an important obstacle to commercialization of BLG, and overcoming commercialization obstacles is an important overall objective of the MISTRA BLG program as a whole. Importantly, at a technical level the modelling work associated with the mill integration and systems analysis is an effective (technically and cost-wise) way to identify and help anticipate and solve problems that are otherwise likely to arise with introduction of BLG at a mill. Mill modelling also provides the basis for preliminary economic assessments that are essential for understanding the potential of alternative process modifications. The key tool to be used in the non-BLG aspects of WP-3 is whole-mill modelling, together with economic analysis, building in part on model development and validation and techno-economic analysis efforts in Phase I (see discussion of SP-7 in Phase I).

Scientific quality and approach

The non-BLG aspects of WP-3 include two proposed sub-packages (SP):

- SP-1 focuses on establishing and quantifying performance (including yield gain and fiber properties) of softwood and hardwood fiber line process configurations that could be implemented when BLG is introduced.
- SP-2 focuses on understanding the whole-mill energy consequences of integrating BLG into different types of mills and external heat sinks (e.g., district heating). Analysis under different future scenarios of product mixes, energy prices, policies in place, and other parameters affecting mill economics.

The primary tool to be used in this analysis is the whole-mill model developed during Phase I (see Phase I, SP-7 discussion). This tool has been shown during Phase I to be able to provide very useful results.

The BLG-specific aspects of WP focus on anticipating (and solving) a potential technical issue with BLG and on examining a potential techno-economic opportunity created with BLG. The BLG-specific aspects of WP-3 include two proposed SPs:

- SP-3 focuses on identifying trace materials that may enter the BLG's post-quench liquid (green liquor) and determining the impact these materials may have on the subsequent wet processing steps, including white liquor preparation and counter-current condensation. The work will also explore alternative routes for removing the trace materials from the green liquor.
- SP-4 will evaluate the technical and economic potential of using pressurized causticizing with BLG, taking advantage of the BLG operation at elevated pressure. Current concepts for BLG implementation assume conventional (atmospheric-pressure) causticization. Causticizing at pressure may provide some technical and economic benefits.

The approach to be used in these sub-projects builds on the global BLG (and associated whole-mill) modelling effort developed in Phase I (SP-7) and in WP-4 of the Phase II effort.

Work Package 4: Process Modelling

Project Leader: Magnus Markland, ETC

Relevance

WP-4 encompasses process modelling (and associated database development) activities associated specifically with the BLG. The work aims to refine and (importantly) validate with data several of the models whose initial development was done during Phase I. The importance of successful modelling to achieving the overall objectives of the MISTRA BLG program have been noted earlier (see discussion of Phase I activities).

Scientific quality and approach
There are four main sub-projects within WP-4.

SP-1 aims to improve and expand the global BLG model that is currently implemented in the larger model of the full pulp mill (see WP-3). In particular, this effort will include incorporating two modifications based on empirical data generated in other WPs: green liquor inorganic chemistry (WP-5), which will enable prediction of accumulations and deposit formation from non-process elements in the BLG plant, and organic components (tar, WP-1) to be able to predict the fate of these components. It will also include converting the global BLG model from a steady-state model to a dynamic model to be able to predict performance during start-up and off-design operation. The refined global model will be validated by comparing results against data collected from the operation of DP-1. Having a refined and validated global BLG model is important for accurate whole-mill modelling, the importance of which for commercialization of BLG has been discussed under WP-3. Having a dynamic global model may be useful to help debug difficulties encountered during transient or off-design operation of the DP-1 plant, but the utility for the whole-mill modelling activities (WP-3) is not obvious.

SP-2 aims to refine and validate the CFD models of the DP-1 hot section and quench on the basis of experimental data to be collected using the pressurized laminar entrained flow reactor at the IPST in USA. The importance of these CFD models for facilitating scale up has been noted in the review of Phase I results. During Phase II, results from the model will be compared with data collected from experiments at IPST and in the DP-1, and further adjustments will be made to the models if needed to improve accuracy. The detailed task 4.2 discussion on page 48 does not explicitly say that DP-1 data will be used for validation, but discussion elsewhere suggests this will be the case. The Scientific Review Panel believes that it is essential that DP-1 data be used for this purpose.

SP-3 is designed to build the most up-to-date, reliable, consistent, and transparent database of thermodynamic properties for all components relevant to smelt and gas phase modelling. The database will include properties developed during Phase I and Phase II work, as well as literature data where those are the best available. The database will be used for calculations by all models developed during Phase II. This should ensure the most accurate calculations possible, and it will facilitate comparisons between results from different models by eliminating one possible source of discrepency. The transparency of the database will enable it to be easily updated as future improved data become available. SP-3 also includes validation of the database against DP-1 data by use of the simple 4-box model developed for this purpose in Phase I work.

SP-4 is designed to understand the extent and nature of the formation and destruction of products of incomplete gasification (PIG) for purposes of developing a simple model of PIG mechanisms to be incorporated into the CFD model of the hot reactor. Furthermore, experiments will be done (using methods developed in WP-1) to measure the vapor-liquid equilibrium (VLE) of PIG in the quench water. A simple VLE model will be developed to be incorporated into the CFD models of the quench and condenser sections of the BLG system. Tar (PIG) production in biomass gasifiers is a major concern and operational problem. The extent of tar production in the Chemrec gasifier is not well known at this stage, but preliminary data suggest that tar production may be quite limited due to the relatively high operating temperatures and catalytic effect of alkali species found in kraft black liquor. The simplified modelling work suggested in task 4.4 is needed for the CFD modelling work. The data needed for simplified modelling can be obtained from existing knowledge associated with biomass gasification.

Work Package 5: Underpinning process chemistry

Project leader: Anders Nordin, Umea University

Relevance

The fundamental data improvement for inorganic and especially sulfur species have been successful, with strong relevance for the research and development program for the HT BLG process. The remaining activities in the area are important to conclude .

That includes smelt chemistry as well as material studies.

The need for new kidney solutions to get rid of contaminants was pointed out during phase 1 and is still important. The results of borates autocausticizing experiments from Phase I do not support that this is important to develop further. After planned additional testing in DP-1 a final conclusion can be drawn.

In the area of PIG (products of incomplete gasification) the focus on "tar" does not seem to be justified by earlier results. Additional testing in DP-1 will answer whether such a focus after all is justified.

Some testing on soot and char formation and alkali content and reactivity could be of interest if this problem should be indicated when running DP-1 at full load and pressure.

To extend the fundamental testing to hydrocarbons should be justified by similar sensitivity analysis as earlier done on the inorganics. The quality of fundamental data is probably better for hydrocarbons as they are in widespread use in several types of industrial applications.

Scientific quality and approach

The approach in phase one related to inorganics is proven and the results have significantly improved the understanding of the process. Some items such as smelt chemistry and material problems need further attention and the methods suggested seem convincing and effective.

The new areas for organics and PIG needs verification in the DP-1 tests to be able to put priority on the right problem. Judging from today's data "tars" may not be a big problem and detailed small-scale studies are not justified.

If the "tar" composition reported at the hearing (from the Karlstad tests) with very low levels 100 ppm and with 90% as naphthalene are correct, that tells a lot about the reaction scheme in HT BLG. Thermal tar cracking leads finally to formation of soot that is difficult to convert due to low reactivity. The thermal route also yields a widespread distribution of heavy and complicated hydrocarbons including PAH. The catalytic route for tar conversion first eliminates the heavy tars and reduces the number of heavy compounds. Finally naphthalene and BTX are the remaining most stable compounds. The presented results indicate that the HT BLG, despite short residence time but due to the high temperature and the high ash content with alkaline species, essentially proceeds through the catalytic route.

If the DP-1 test proves tar to be of importance and of a more complicated nature cooperation should be established with similar research in the biomass gasification area e.g. RIT in Sweden, VTT in Finland or ECN in Holland.

Comments to individual subtasks:

ST 5.1 Any start of more detailed work should wait until DP-1 results are available.

ST 5.2 Important to finalize earlier successful work.
ST 5.3 Put priority on inorganic and sulfur reactions.
ST5.4 Any new information on these issues is important.
ST 5.5.1 Important question that needs new answers.
ST 5.5.2-3. Borates should be given low priority unless new indications show better promise for this technology for HT BLG.
ST 5.5.4 Important tasks for all partners in the research project.
ST 5.6 Improved data for the new regime of operation is important.
Special attention should be taken to feed back any results from the DP-1 results to the fundamental program for further guidance and new priorities.

6. Program Deliverables

Deliverables and milestones are available in the work packages but not at the program level. In the program plan for 2007-2009 deliverables and milestones with timetable should be developed.

7. Budget

The review panel has not the full picture of the resources available to the program. The above discussions of individual work packages provides some input on prioritization should it be necessary to reduce budget from the requested amount. It should be noted, however, that this unique technology is very close to commercialization and should be resourced for success. Furthermore it is the review panel's opinion that this program fulfills all of the MISTRA criteria for support.

8. Recommendations and Priorities

The pilot plant (DP-1) in Pitea is unique in the world and provides an opportunity for rapid commercialization and deployment of the high temperature, pressurized BLG technology. The overall goals of the MISTRA BLG program are to:

- Remove obstacles to commercialization of BLG
- Develop sound scientific understanding of high temperature BLG
- Try to predict possible future problems before they occur

The highest priority should be given to the following:

- Operation and measurements on DP-1
- Facilitating scale up and process optimization
- Understanding integration with present and future pulping and causticizing cycles
- Identifying containment materials for BLG components
- Understanding high temperature chemistry and kinetics

With respect to the BLG II proposed program the Scientific Review Panel has the following comments for consideration:

The uniqueness of the DP-I pilot facility should be exploited. Therefore, Work Package 1 is extremely important and critical to the above stated goals. Access by the researchers to the pilot facility is necessary and a key strength of the program. Measurement techniques and data gathering are essential, and given the very hostile environment of the reactor these activities will be very difficult. The panel believes that the resources proposed for this work package may be underestimated.

Success in Work Package 1 is meaningless unless the data are utilized to advance the program. Therefore, Work Package 2 is equally important. The panel believes that tasks 2.1 and 2.2 are well conceived and should succeed in achieving their respective goals provided that the Panel's concern of selecting only one operating condition in task 2.1 is taken into consideration. Tasks 2.3 and 2.4 are also very important, but to be successful they should be reconsidered and strengthened. This is extremely important in that the results here will have significant implications in the development of useful models which are being developed in Work Package 4.

Work Package 3, particularly tasks 3.1 and 3.2, are viewed by the panel as well conceived and relevant because they promise to provide an understanding of potential mill-wide impacts and opportunities when BLG is introduced. Without such understanding, mill owners will be reluctant to invest in commercial BLG systems. Also, the results of these tasks, when appropriately presented, offer the potential to deliver useful understanding for government policy makers to make better informed decisions, e.g., regarding the positive environmental impacts of BLG adoption as well as incentives that might be provided to encourage adoption.

Work Package 4 is also well conceived and relevant. A critical element for the success of this package is the availability of experimental data from the DP-1 facility that can be used to refine and validate the models.

Work package 5 represents advancements in fundamental understanding of high temperature chemistry and kinetics. The panel feels that to some extent there is a trade off between the kind of information obtained in Work Package 1 and Work Package 5. At this time and given the uniqueness of the pilot plant availability the panel feels that the emphasis should be given to Work Package 1. If resource constraints exist Work Package 5 should be carefully focused on only truly essential objectives allowing for essential resources be allocated to Work Package 1. One approach that should be considered is to give initial focus on the inorganic reactions and material issues and put a lower priority on the hydrocarbons until DP-1 shows whether or not this is an issue.

Finally, the Panel wishes to commend the program team and leadership for the successful effort to organize, focus and develop international collaboration in the program. The team spirit and mutual respect among team members is impressive. The significant expertise among a diverse set of people being developed through this program is critical for the future deployment and support of the BLG technology. Successful commercialization and deployment of the BLG technology will make a very significant positive difference in the production of forest based products world wide. The teams support in working to achieve this goal is noted and appreciated.

Appendix 1

BLG, The Black Liquor Gasification Programme

17-19 May, 2006

The Scientific Review Panel

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Appendix 2

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