CLEAN RESOURCES FINAL REPORT PACKAGE

Project proponents are required to submit a Final Report Package, consisting of a Final Public Report and a Final Financial Report. These reports are to be provided under separate cover at the conclusion of projects for review and approval by Alberta Innovates (AI) Clean Resources Division. Proponents will use the two templates that follow to report key results and outcomes achieved during the project and financial details. The information requested in the templates should be considered the minimum necessary to meet AI reporting requirements; proponents are highly encouraged to include other information that may provide additional value, including more detailed appendices. Proponents must work with the AI Project Advisor during preparation of the Final Report Package to ensure submissions are of the highest possible quality and thus reduce the time and effort necessary to address issues that may emerge through the review and approval process.

Final Public Report

The Final Public Report shall outline what the project achieved and provide conclusions and recommendations for further research inquiry or technology development, together with an overview of the performance of the project in terms of process, output, outcomes and impact measures. The report must delineate all project knowledge and/or technology developed and must be in sufficient detail to permit readers to use or adapt the results for research and analysis purposes and to understand how conclusions were arrived at. It is incumbent upon the proponent to ensure that the Final Public Report **is free of any confidential information or intellectual property requiring protection**. The Final Public Report will be released by Alberta Innovates after the confidentiality period has expired as described in the Investment Agreement.

Final Financial Report

The Final Financial Report shall provide complete and accurate accounting of all project expenditures and contributions over the life of the project pertaining to Alberta Innovates, the proponent, and any project partners. The Final Financial Report will not be publicly released.

CLEAN RESOURCES FINAL PUBLIC REPORT TEMPLATE

1. PROJECT INFORMATION:

Project Title:	**Sheath-Core Carbon Fibre Precursor (Carbon Fibre Grand Challenge)**
Alberta Innovates Project Number:	G2020000348
Submission Date:	January 15, 2021
Total Project Cost:	$82,055
Alberta Innovates Funding:	$50,000
AI Project Advisor:	Murray Gray

2. APPLICANT INFORMATION:

Applicant (Organization):	**Chemventive LLC**
Address:	38 Ringfield Road, Chadds Ford, PA 19317, USA
Applicant Representative Name:	John Newport
Title:	Managing Director
Phone Number:	01-610-357-1335
Email:	jflnewport@chemventive.com

3. PROJECT PARTNERS

Please provide an acknowledgement statement for project partners, if appropriate.

RESPOND BELOW

A. EXECUTIVE SUMMARY

Provide a high-level description of the project, including the objective, key results, learnings, outcomes and benefits.

RESPOND BELOW

This project is part of the $15 million Carbon Fibre Grand Challenge targeted to accelerate the production of high strength carbon fibre from bitumen-derived asphaltenes . Currently carbon fibres are made commercially from pitch or polyacrylonitrile. Using pitch first requires its conversion into a different form via chemical and thermal treatment. Whether asphaltene would require prior modification to make carbon fibre was unknown.

Here we investigated the possibility of using a sheath core technology where the oxidized sheath might be expected to provide higher strength during fibre spinning. Additionally we worked on developing an AI driven computer model of the fibre spinning process that can be used to optimize the production of high strength fibres.

Using asphaltene (*Asphaltene Sample Bank Sample S-2*) as is produces very brittle fibres which we found was not improved by asphaltene oxidation. We were however successful in developing an AI driven computer model that will have benefit going forward in the manufacture of high strength asphaltene based carbon fibres.

B. INTRODUCTION

Please provide a narrative introducing the project using the following sub-headings.

- **Sector introduction:** Include a high-level discussion of the sector or area that the project contributes to and provide any relevant background information or context for the project.
- **Knowledge or Technology Gaps:** Explain the knowledge or technology gap that is being addressed along with the context and scope of the technical problem.

RESPOND BELOW

Sector Introduction

The Carbon Fibre Grand Challenge of which this project is a part is a $15 million international competition to accelerate the production of carbon fibre from bitumen-derived asphaltenes . The Carbon Fibre Grand Challenge is part of the broader “Bitumen Beyond Combustion” initiative by Alberta Innovates to further the development of non-combustion products and their production technologies, derived from bitumen contained in Alberta’s oil sands, which are among the world’s largest hydrocarbon resources with proven reserves of approximately 170 billion barrels.

Knowledge of Technology Gaps

The major technology gap is whether it is possible to melt spin asphaltene directly in a viable commercial process and make a carbon fibre precursor that can then be converted by established means into a high strength carbon fibre. Currently carbon fibres are made from either polyacrylonitrile or pitch based fibres. Pitch cannot be used directly to make fibres commercially. Instead it needs to be chemically modified. This project, along with others, will fill the technology gap in this respect for asphaltene

C. PROJECT DESCRIPTION

Please provide a narrative describing the project using the following sub-headings.

- **Knowledge or Technology Description:** Include a discussion of the project objectives.
- **Updates to Project Objectives:** Describe any changes that have occurred compared to the original objectives of the project.
- **Performance Metrics:** Discuss the project specific metrics that will be used to measure the success of the project.

RESPOND BELOW

Knowledge or Technology Description

Our proposal, which was based on the expectation that an oxidized sheath would enhance spinnability of asphaltene fibre and remove the need for a mesophase formation, had two main components. An experimental section aimed at determining the melt viscosity of asphaltene as a function of temperature and flow rate in a capillary viscometer together with looking at the high temperature oxidation characteristics of asphaltene and a theoretical section aimed at developing a model of the fibre spinning process including sub spinnerette radial oxidation so as to allow rapid process optimization.

Updates to Project Objectives

No updates were made to the project objectives

Performance Metrics

Performance metrics were the measurement of rheological and oxidative characteristics of asphaltene and the development of a computer model of the spinning process that included the oxidation of the outer sheath of the fibre in the immediate sub spinnerette zone.

D. METHODOLOGY

Please provide a narrative describing the methodology and facilities that were used to execute and complete the project. Use subheadings as appropriate.

RESPOND BELOW

Laboratory facilities used the following methodologies

Rheometry

Capillary rheometer mimics the fibre extrusion process and can be used to generate melt viscosity data as a function of temperature and flow rate as well as get some information on fibre spinning characteristics.

Oxidation : Thermal gravimetric analysis

Computation:

Hardware used for AI design optimization. (44 core server with 256 GB ramp. NVidia Cuda acceleration card. 4 TB Raid HD array.)

E. PROJECT RESULTS

Please provide a narrative describing the key results using the project's milestones as sub-headings.

- Describe the importance of the key results.
- Include a discussion of the project specific metrics and variances between expected and actual performance.

RESPOND BELOW

Key results were that :

1 Asphaltene can be extruded in the 280 – 300 deg C range but gives a very brittle difficulty extensible extrudate.

2 Oxidation of the asphaltene does not enhance extensibility. Asphaltene undergoes significant weight loss at temperatures over 300 deg C in air.

3 Plasticization of the asphaltene allows easy fibre drawdown but does not improve brittleness.

4 A sophisticated highly accurate AI driven computer model of the fibre spinning process was developed that can be used to optimize any fibre spinning process. A particularly useful feature is the methodology can be used to minimize the phenomena of draw resonance that leads to fibre diameter periodic variation along the fibre length. This impacts the ultimate fibre strength and so its elimination is of key importance.

F. KEY LEARNINGS

Please provide a narrative that discusses the key learnings from the project.

- Describe the project learnings and importance of those learnings within the project scope. Use milestones as headings, if appropriate.
- Discuss the broader impacts of the learnings to the industry and beyond; this may include changes to regulations, policies, and approval and permitting processes

RESPOND BELOW

From our perspective the key learning is that asphaltene will require some type of modification in order to use it as a feedstock for the production of high strength carbon fibres. This is similar to pitch based carbon fibres where pitch has to be first converted to a mesophase in order to have a commercially viable fibre manufacturing process.

Another key learning is that we have developed an AI driven computer model of the fibre spinning process that can be used to design an optimum process for the manufacture of high strength fibres.

G. OUTCOMES AND IMPACTS

Please provide a narrative outlining the project's outcomes. Please use sub-headings as appropriate.

- **Project Outcomes and Impacts:** Describe how the outcomes of the project have impacted the technology or knowledge gap identified.
- **Clean Energy Metrics:** Describe how the project outcomes impact the Clean Energy Metrics as described in the *Work Plan, Budget and Metrics* workbook. Discuss any changes or updates to these metrics and the driving forces behind the change. Include any mitigation strategies that might be needed if the changes result in negative impacts.
- **Program Specific Metrics:** Describe how the project outcomes impact the Program Metrics as described in the *Work Plan, Budget and Metrics* workbook. Discuss any changes or updates to these metrics and the driving forces behind the change. Include any mitigation strategies that might be needed if the changes result in negative impacts.
- **Project Outputs:** List of all obtained patents, published books, journal articles, conference presentations, student theses, etc., based on work conducted during the project. As appropriate, include attachments.

RESPOND BELOW

Project Outcomes and Impacts

Project findings contribute to the knowledge gap relating to the spinnability of AOA into carbon fibre precursors

Clean Energy Metrics

Asphaltene , like other bitumen derived products, is currently often burnt for fuel value acting as a source for greenhouse gas emissions. Using it instead to make high value products such as carbon fibres favourably impacts clean energy metrics.

Program Specific Metrics

Our original premise that a sheath core fibre structure embodying an oxidized sheath would remove the need for a mesophase conversion of asphaltene was not borne out.

Project Outputs

Currently no patents, journal articles or presentations have been written or conducted

H. BENEFITS

Please provide a narrative outline the project's benefits. Please use the subheadings of Economic, Environmental, Social and Building Innovation Capacity.

- **Economic:** Describe the project's economic benefits such as job creation, sales, improved efficiencies, development of new commercial opportunities or economic sectors, attraction of new investment, and increased exports.
- **Environmental:** Describe the project's contribution to reducing GHG emissions (direct or indirect) and improving environmental systems (atmospheric, terrestrial, aquatic, biotic, etc.) compared to the industry benchmark. Discuss benefits, impacts and/or trade-offs.
- **Social:** Describe the project's social benefits such as augmentation of recreational value, safeguarded investments, strengthened stakeholder involvement, and entrepreneurship opportunities of value for the province.
- **Building Innovation Capacity:** Describe the project's contribution to the training of highly qualified and skilled personnel (HQSP) in Alberta, their retention, and the attraction of HQSP from outside the province. Discuss the research infrastructure used or developed to complete the project.

RESPOND BELOW

Economic

The ability to use abundant Alberta Oil Sands asphaltene to make high strength carbon fibres will have a positive impact on job growth and overall income in the Province as production facilities are built and come on stream. In their wake will come other downstream manufacturers

Environmental

Currently bitumen derived products such as asphaltene are mainly burnt for fuel value. Using them for the production of a high value product such as carbon fibre will have a major impact on greenhouse gas emissions and air quality in general.

Social

A positive impact can be expected

Building Innovation Capacity

A positive impact can be expected

I. RECOMMENDATIONS AND NEXT STEPS

Please provide a narrative outlining the next steps and recommendations for further development of the technology developed or knowledge generated from this project. If appropriate, include a description of potential follow-up projects. Please consider the following in the narrative:

- Describe the long-term plan for commercialization of the technology developed or implementation of the knowledge generated.
- Based on the project learnings, describe the related actions to be undertaken over the next two years to continue advancing the innovation.
- Describe the potential partnerships being developed to advance the development and learnings from this project.

RESPOND BELOW

To be determined

J. KNOWLEDGE DISSEMINATION

Please provide a narrative outlining how the knowledge gained from the project was or will be disseminated and the impact it may have on the industry.

RESPOND BELOW

The AI driven computer model of the fibre spinning process can be used to accelerate the introduction of a commercial process for carbon fibre production based on asphaltene.

K. CONCLUSIONS

Please provide a narrative outlining the project conclusions.

- Ensure this summarizes the project objective, key components, results, learnings, outcomes, benefits and next steps.

RESPOND BELOW

The properties of asphaltene prevent it from being satisfactorily spun as is into a carbon fibre precursor due to the extreme brittleness of the fibre. Like pitch it is expected that asphaltene will require some type of modification to produce a more robust fibre.

Oxidation of the asphaltene does not improve the situation and so our original premise that a sheath core fibre structure would remove the need for a mesophase conversion of asphaltene was not borne out.

We were successful in developing an AI based model for the fibre spinning process that allows process optimization with input variables obtained from just a few actual monofilament spinning experiments. Just one benefit of the model is it predicts the phenomenon of draw resonance where the thread line diameter changes (pulses) with time The variation in fibre diameter then persisting throughout the rest of the process and limiting the ultimate strength of the fibre bundle. Thus the model can be used to design a commercial spinning process that minimizes draw resonance.