# Advancing Bio-Based Chemicals and Next-Generation Fuels from Montana's Agricultural Crops

Quarterly Report

Submitted by:

December 2015

Jessica Windy Boy Director and Lead Principal Investigator Advanced Fuels Center Montana State University-Northern

Montana State University - Northern Advanced Fuels Center



# 1. Personnel Recruitment and Employment

# 2. Equipment Purchased

Billings City College is currently seeking bids for a pelletizer. MSU-Northern is not buying any equipment with MREDI funding.

# 3. Progress towards Meeting Milestones

**OBJECTIVE 1:** Evaluate the environmental life cycle analysis (LCA) impacts and technoeconomic feasibility of green diesel and bio-jet fuel (next-generation fuels) and high-value added chemicals (bio-based chemicals).

Key Milestones	Schedule	Status of Deliverables
1.1 Development of a thorough unit process analysis and life cycle inventory of the entire camelina-to-next-generation fuels/bio-based chemicals process chain.	July 1, 2015 to July 1, 2016 (20% complete)	<ul> <li>LCA software called SimaPro and Crystal Ball Financial Modeling software have been ordered.</li> <li>Preliminary data on extracting oil from camelina seeds via mechanical and chemical extraction methods has been collected.</li> </ul>
1.2. Comparative assessment of "cradle- to-gate" life cycle impacts of camelina- to-next-generation fuels/bio-based chemicals.	July 1, 2016 to January 1, 2017	Not started
1.3. Evaluation of tech-economic feasibility of camelina-to-next generation fuels/bio-based chemicals via life cycle costing (LCC).	January 1, 2017 to July 1, 2017:	Not started

Table 1. Key milestones	s and status	of Objective 1.
-------------------------	--------------	-----------------

### *Explanation of variance:*

Not applicable.

**OBJECTIVE 2:** Propose and validate the mechanism of producing high-octane number chemicals (e.g., alkylated aromatics) from camelina.

Key Milestones	Schedule	Status of Deliverables
2.1 Validation of the mechanism of producing high-octane number chemicals from camelina.	July 1, 2015 to December 1, 2015 (95% complete: Please see the explanation below)	<ul> <li>A cryogenic (CO<sub>2</sub>) cooling system has been added to the center's GC/MS instrument. This allowed us to identify the composition of aviation gasoline.</li> <li>A new mechanism of converting camelina to high-octane chemicals number was proposed and validated through experiments.</li> <li>Experimental results were presented at the 28<sup>th</sup> Annual Fall Social, American Chemists' Society Montana Section.</li> <li>A proposal entitled, "Development of Renewable High-Octane Blend Component for Aviation Gasoline" was submitted to FAA and it is currently under review.</li> </ul>
2.2. Optimum ratio of camelina-derived alkylated aromatics and unleaded avgas with desired anti-knock value identified.	December 1, 2015 to October 1, 2016	Not started
2.3. Certification of the newly- formulated unleaded avgas.	October 1, 2016 to June 30, 2017	Not started

Table 2. Key milestones and status of Objective 2.

#### *Explanation of variance:*

The research team has successfully confirmed the mechanism of producing high-octane number chemicals. Moreover, an alternative catalyst, which is environmentally-friendly and abundantly available, was discovered to be also effective in producing high-octane number chemicals from camelina oil. This discovery lead to more experiments and more data. Thus, we postponed publishing our findings to science journals. We expect to have an article published by the next reporting period. This action will not affect the subsequent tasks.

**OBJECTIVE 3:** Develop a novel and robust heterogeneous Grubbs catalyst that achieves efficient conversion of natural oils to next-generation fuels and bio-based chemicals.

Key Milestones	Schedule	Status of Deliverables
3.2 Synthesis of a silica- supported polymeric Grubbs catalyst for olefin metathesis of natural oils.	July 1, 2015 to June 30, 2016 (50% Complete)	<ul> <li>Second Generation Grubbs catalysts are built on N-heterocyclic carbene (NHC) ligand complexed with Ruthenium (Ru) alkylidene complex. In this section we want to synthesize silica-supported polymeric Grubbs catalyst for olefin metathesis. The work consists of several steps: (i) Ruthenium (Ru) alkylidene complex synthesis; (ii) synthesis of N-Heterocyclic carbene monomer; (iii) synthesis of N- Heterocyclic carbene polymer; (iv) complexation of ruthenium (Ru) alkylidene complex with polymer to afford polymeric Grubbs Catalysts. (v) If this process work, NHC polymer will be grown on the surface of silica and hence polymeric Grubbs catalysts on silica surface</li> <li>Ruthenium (Ru) alkylidene complex has been synthesized and characterized.</li> <li>Styrene substituted N-Heterocyclic carbene monomer has been synthesized and characterized</li> <li>Polymer of NHC ligand has been synthesized Characterization of the polymer is under going.</li> </ul>
3.1 Synthesis of a novel silica- supported Grubbs catalyst for olefin metathesis of natural oils	July 1, 2016 to December 31, 2016	Not started
3.3. Comparative analysis of the two heterogeneous Grubbs catalysts.	January 1, 2017 to June 30, 2017	Not started

Table 3. Key milestones and status of Objective 3.

### Explanation of variance:

Second Generation Grubbs catalysts are built on N-heterocyclic carbene (NHC) ligand complexed with ruthenium (Ru) alkylidene complex. Simple hypothesis: polymer of the NHC ligand complexed with ruthenium (Ru) alkylidene complex will also give second generation Grubbs catalysts. Since this method is relative easy and straight forward, the research team started first with polymeric Grubbs catalyst. In this case reactivity tests and characterization of the catalyst will be relative easy compared to silica bound catalyst. Once the fundamental studies with the polymeric catalyst process is carried out and the

process become successful, Grubbs catalyst both polymeric (objective 3.2) and second generation (objective 3.2) will be synthesized on silica surface.

**OBJECTIVE 4:** Develop and prepare a design study documenting an optimum process configuration and economic analysis for medium- and large-scale pelletizing plants for camelina meal (next-generation fuels).

Key Milestones	Schedule	Status of Deliverables
4.1 Development of an optimized process for fuel pellet production from camelina meal and manufacture a range of pellet compositions to verify producibility.	Summer 2016 (30% complete)	<ul> <li>Started student research on optimizing oil extraction from camelina seeds using screw presses.</li> <li>Collected 400 lbs of dry grass clippings that will be used for the project. Additional sources of grass clippings has been also identified.</li> </ul>
4.2. Testing of products in a range of commercially-available multi-fuel pellet stoves and identification of potential markets to determine product price including a fish food for export.	Winter 2017	Not started
4.3. Preparation of study design for 40,000 to 500,000 ton per year pelletizing plant with economic analysis.	Summer 2017	Not started

Table 4. Key milestones and status of Objective 4.	
--	--

### *Explanation of variance:*

Not applicable.

# 4. Budget Summary

### 710707 MSUN Bio-Energy OTO FY16 as of 11/30/15

		Budget	YTD	Remaining
61100/61200	Salaries/Wages	130,309.00	42,491.17	87,817.83
61400	Benefits	40,903.95	15,662.37	25,241.58
62100	Contracted Services	3,000.00	-	3,000.00
62200	Supplies	12,000.00	3,110.44	8,889.56
62300	Communications	1,400.00	1,032.93	367.07
62400	Travel	5,000.00	222.76	4,777.24
62500	Rent	-		-
62700	Repair & Maintenance	-		-
62800	Other	6,967.00		6,967.00
62827M	Indirect Costs	-		-
		199,579.95	62,519.67	137,060.28

Excludes TIAA-CREF 1% HB95