

# Combustion Chemistry of Biodiesel for Use in Urban Transport Buses: Experiment and Modeling



MNTRC Report 12-17



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REPORT 12-17

**COMBUSTION CHEMISTRY OF BIODIESEL FOR  
USE IN URBAN TRANSPORT BUSES:  
EXPERIMENT AND MODELING**

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<b>16. Abstract</b>  <p>Biofuels, such as biodiesel, offer benefits as a possible alternative to conventional fuels due to their fuel source sustainability and reduced environmental impact. Before they can be used, however, it is essential to understand their physical properties, combustion chemistry, and characterization of the exhaust due to a number of issues associated with fuel properties—for example, a lower heating value and higher cloud point than regular diesel. High viscosity of biodiesel may lead to poor atomization of the fuel spray and inaccurate operation of the fuel injectors, so, it may cause fuel injector problems. Biodiesel may produce high NOx emissions. Depending on the feedstocks and blending ratios used to produce the fuel, variations in chemical properties may also be an issue.</p> <p>During this study, physical properties such as flash point, cloud point, and kinematic viscosity of different blends (B0, B10, B20, B50, and B100) were measured on three different feedstocks (soybean methyl ester or SME, tallow oil, or TO, and waste cooking oil, or WCO) while ultra-low sulfur diesel (ULSD) was used as base fuel. The research applied the standard methods of the American Society for Testing and Materials (ASTM). For the study of combustion chemistry and characterization of the exhaust, various tests, such as gravimetric analysis, elemental analysis, elemental carbon/organic carbon (EC/OC) analysis, and gas chromatography (GC) analysis, were conducted for PM emission samples collected from buses, as well as from the laboratory setup. In the field, emission samples were collected for both hot and cold idle conditions.</p> <p>Gravimetric analysis showed a decrease of 17% in PM emissions from the transit buses running on B20 compared to ULSD (B0). A total of eleven elements were detected in the exhaust samples collected from the laboratory experiments, and fifteen elements from the field experiments. Calcium (Ca), sodium (Na), and iron (Fe) were the major elements. The results also indicated that the use of biodiesel could effectively reduce EC and increase the portion of OC/EC emissions. Positive matrix factorization (PMF) was used to identify all possible sources of the elements from the transit buses. A simple chemical model was also proposed on PM formation from transit buses, as well as the emission from the laboratory experiments. The emission of carbon was also investigated, and the results confirmed that lower emissions of CO and CO2 are related to lower ratios of carbon to oxygen in biodiesel fuels compared to ULSD.</p>			
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## EXECUTIVE SUMMARY

Biofuels, such as biodiesel, are of increasing interest as an alternative to conventional fuels because they offer the long-term promise of fuel-source sustainability and reduced environmental impact. But biodiesel combustion chemistry and characterization of the exhaust need more in-depth study due to the number of issues observed in emissions and applicability of pure biodiesel. Some of these major issues are lower heating value compared to regular diesel, less favorable cloud point, lower volatility, higher viscosity which causes poor combustion, material incompatibility, possibly high emission of NO<sub>x</sub>, filter clogging in vehicles when used in pure form, and variation of chemical properties between different feedstocks and blends.

Combustion of biodiesel from various types of feedstock, such as soybean methyl ester (SME), tallow oil (TO), and waste cooking oil (WCO), in variety of volume percent blends (B00, B20, B50, and B100) was investigated using a bench top combustion chamber in a laboratory setting. Ultra-low-sulfur diesel (ULSD) was used as base fuel. Different combinations of combustion temperature and pressure were applied to investigate their effects on emissions. In addition, physical properties (flash point, cloud point, and kinematic viscosity) of all biodiesel blends were measured following the American Society for Testing and Materials (ASTM) standard methods.

Particulate matter (PM) samples were collected through field tests to investigate the source of elements in the emission gases released by buses. Ten different transit buses running on B20, which contains 20 vol% of SME with 80 vol% ULSD, were used for the field study. A similar procedure was followed to collect and analyze PM from the laboratory combustion experiments to determine precisely which elements are from biodiesel fuels. A total of eleven inorganic and metal elements were detected in the laboratory experiments, while fifteen elements were observed in field experiments. Calcium (Ca), sodium (Na), and iron (Fe) were the major elements found in the PM emissions in both the field experiments—77 – 85 weight percent (wt%)—and the lab experiments—up to 90 wt%.

Based on gravimetric analysis, PM emissions significantly decreased by less than 17% on average when using B20, and newer transit buses showed a greater PM reduction (more than 98% on average) than old buses when using ULSD. For both hot and cold idle tests, a substantially high reduction in total particulate matter (TPM) was observed, and the maximum PM concentrations for ten different buses under hot and cold idle conditions were 2.77 and 5.59 µg/m<sup>3</sup>, respectively.

To complete PM characterization, elemental carbon (EC) and organic carbon (OC) analyses of the collected PM from field tests were carried out by an accredited analytical laboratory. OC/EC analyses showed that more OC was emitted during cold idling (>80%) than in hot idling (>65%). Furthermore, the OC/EC ratio was found to be greater for new buses with catalytic converters (9.57 – 13.37) than for old buses without converters (1.85 – 4.55). Finally, positive matrix factorization (PMF) showed that four sources—oil (including fuel and engine oil), lubricant, engine parts, and ambient conditions—contributed heavily to the generation of PM in the exhaust.

Laboratory test results indicated that when the volume percent of biodiesel increased in biodiesel blends with regular diesel, then combustion temperature and pressure linearly increased. The high oxygen content of biodiesel is thought to be the reason for this increase at the tested combustion temperature and pressure, which also is thought to contribute to the reduction of PM. The high oxygen content of biodiesel improves the oxidation process of nascent PM and reduces its production. The results also confirmed that better combustion, with less emission of PM, occurred in hot idle mode than in cold idle mode. The effect of higher temperature in hot idle mode is thought to be another explanation for the PM reduction, due to changes in physical properties at high temperature. Hot idle samples are the PM samples collected during the nighttime when the buses have been returned to the garage from a regular route. Cold idle samples were collected in the morning before the buses left the garage.

The emission gas was analyzed using gas chromatography (GC) to measure concentrations of emission components in the exhaust. This document reports the emission characteristics of biodiesel fuels and comparison with ULSD and discusses the effect of temperature and pressure. In addition to the experimental results, simple kinetic models were proposed to better understand the formation mechanism of PM and to predict the concentrations of PM and other combustion components.

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## I. INTRODUCTION

### PARTICULATE MATTER

Environmental and health concerns related to particulate matter (PM) have gained increasing attention in the past few decades because PM is one of the most recognized pollutants in urban areas. Particles emitted by different sources (primary and secondary) have been examined with great interest due to their abundance in the atmosphere and the negative effects on human health (heart diseases, respiratory ailments, and carcinogenic effects). Children, the elderly, and those with existing heart or lung disease, asthma, or other respiratory problems, are most sensitive to the health effects of breathing fine particles. Children are more vulnerable to air pollution because they breathe 50 percent more air per pound of body weight than do adults.<sup>1</sup> The most well-known contributors of PM in urban areas are:<sup>2</sup>

- Road-traffic-related exhaust and non-exhaust emissions
- Stationary sources of primary particle formation, such as power plants, metal industries, mines, etc.
- Secondary particle formation due to atmospheric oxidation of sulfur dioxide (SO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), and volatile organic carbons (VOCs). Natural components, such as sea salt, re-suspended soil, and dust are also known to contribute to secondary particle formation.<sup>3</sup>

The shape, size and concentration of the particles have a direct relationship to the risk assessment for human health.<sup>4</sup> These fine and ultrafine particles of PM have higher specific surface areas and toxic effects than coarse particles. Because the deposition efficiency is related to the size of particles, smaller particles can easily be inhaled and deposited in the respiratory tract and alveolar region. As a result, they are more likely to cause respiratory diseases.<sup>5-7</sup>

Emission characteristics of diesel-powered vehicles are recognized as a major contributor to PM generation.<sup>8,9</sup> PM contains a number of components, including acids, organic chemicals, metals, and soil or dust particles. The United States Environmental Protection Agency (USEPA) is concerned about particles that are 10 micrometers or smaller in diameter because those are the particles that generally pass through the throat and nose and enter the lungs. Diesel particles consist of an agglomeration of primary carbon particles and condensed organic compounds, sulfate, and metallic ash.<sup>10</sup> In the past few years, significant efforts have been taken to reduce particle emissions, either by replacing diesels with alternative fuels (such as biodiesel) or through engine modifications.

### BIODIESEL STUDY

In several studies, environmental benefits associated with biodiesel were investigated, and biodiesel was regarded as a viable replacement for petroleum-based diesel fuels. The majority of these studies note that PM produced from biodiesel was low in comparison with

PM generated from regular diesel.<sup>11-26</sup> There are few studies that show an increase in PM emitted from vehicles running on biodiesel.<sup>26-28</sup> The USEPA reported PM reduction when using a B20 biodiesel fuel, which is composed of 20 vol% biodiesel and 80% ULSD.<sup>4</sup> In addition, biodiesel emitted less carbon monoxide (CO), total unburned hydrocarbon, soot (solid carbon fraction of PM), and total PM mass than conventional fuels. Table 1 presents the physical and chemical properties of pure biodiesel (B100) and ULSD.

**Table 1. Key Physical and Chemical Properties of ULSD and Biodiesel**

Physical/Chemical Property	ULSD	Biodiesel (B100) <sup>b</sup>
Density/15 °C (kg/m <sup>3</sup> )	820-850	870-890
Kinematic viscosity/40 °C (cSt)	1.9	1.9-6.0
Cetane number (CN)	40	47 min
Heating value (kJ/kg)	~43000	36500-39500
Oxygen content (% weight)	0	10-12
Sulfur content (ppm)	11 max	0.05 max
Air fuel equivalence ratio	~15	12.5 <sup>a</sup>
Latent heat of evaporation (kJ/kg)	265	230 <sup>a</sup>
Molecular weight (kg/kmol)	~170	290 <sup>a</sup>
Surface tension/40 °C (N/m)	0.026	0.0285 <sup>a</sup>
Boiling point (°C)	180-360	345 <sup>a</sup>
Bulk modulus of elasticity (bar)	16000	17500 <sup>a</sup>
Flash point (°C)	55	130 min
Ash wt. %	0.01 max	0.02 max
Ca and Mg combined	NR <sup>c</sup>	5ppm max

<sup>a</sup> Average values.

<sup>b</sup> SME.

<sup>c</sup> Not reported.

As shown in Table 1, one of the most important differences between biodiesel and ULSD is the relatively high CN of biodiesel. CN is one of the parameters that determine the quality of fuel, and is the equivalent of octane number for gasoline. A high CN means a fuel ignites rapidly with a short ignition delay after injecting the fuel into an engine. The high oxygen content of biodiesel is another important difference. Other properties, such as flash point and viscosity, have significant effects on engine performance as well as on emissions. More details on these physical properties and their effects on emissions are discussed later. Biodiesel has lower sulfur than most petroleum-based diesel, including ULSD. Sulfur content in biodiesel is very low (<1%), and virtually no SO<sub>x</sub> is produced during combustion.<sup>29-31</sup> The high oxygen content of biodiesel allows it to burn more completely; as a result, fewer unburned fuel emissions are produced. Due to the small number of carbon atoms in biodiesel, the heating value of biodiesel is lower than that of ULSD.

Biodiesel has received considerable attention for its potential as an alternative source of fuel for the transportation sector. The consumption of biodiesel has increased dramatically since early 2000, as biodiesel was considered ready-to-use renewable energy, providing a solution to decrease greenhouse gas emissions. It helps stabilize the price of fossil fuel

and enhances energy security. For these reasons, biodiesel has gained prominence as an attractive fuel in recent years. It is expected that biodiesel will be used extensively in the future because it offers the following characteristics:<sup>32,33</sup>

- Renewable and non-petroleum-based
- Lower greenhouse gas emissions
- Less toxic
- Biodegradable
- Lower emissions of PM, CO, hydrocarbons (HCs), and other air toxins
- Minor (or no) modifications needed for traditional compression ignition engine

Some of the limitations of biodiesel include:

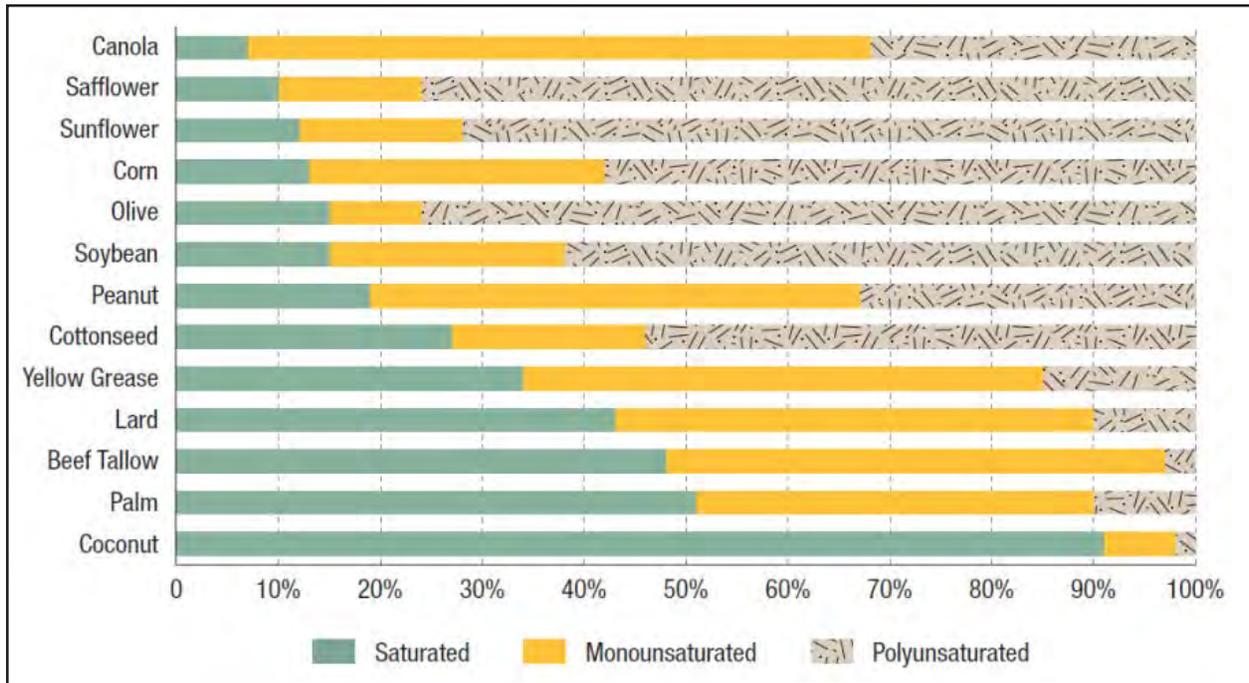
- Lower heating value, less favorable cloud point (mostly positive in pure), lower volatility, and higher viscosity, resulting in poor combustion compared to regular diesel
- Lower storage stability than regular diesel and material compatibility issues
- Potentially high emissions of NO<sub>x</sub>
- High manufacturing cost
- Variation in chemical properties due to differences in feedstock

Biodiesel is obtained from various feedstocks, such as plant oils, animal fats, and waste cooking oils. Until recently, most biodiesel was produced from plant oils, such as soybean oil (USA), rapeseed oil (EU), or palm oil (Asia). Recently the range of feedstocks has been extended to many other oils, fats, and waste oils such as mustard, coconut, peanut, olive, sesame, and safflower oils, algae, fungi, bacteria, molds, yeast, and even trap greases.<sup>32</sup> Today, biodiesel fuels are produced commercially from the following feedstocks:<sup>32</sup>

- Animal fats: edible, inedible, and all other variations of tallow, lard, choice white grease, yellow grease, poultry fats, and fish oils
- Plant oils: soy, corn, canola, sunflower, rapeseed, safflower, and cottonseed
- Recycled oils and greases: waste cooking oils (WCOs), used motor oils, and greases

The fats and oils typically used for biodiesel production are chemically very similar and contain approximately 10 common types of fatty acids, each having 12 to 22 carbons in their molecular structure, more than 90% of which contain 16 to 18 carbons. These chains are saturated, monounsaturated, and polyunsaturated. Each feedstock is distinguished from

the others by its unique proportions of saturated, monounsaturated, and polyunsaturated fatty acids, as shown in Figure 1.<sup>32</sup> SME is rich of polyunsaturated and lean of saturated fatty acids.



**Figure 1. Composition of Various Biodiesel Feedstocks in Order of Increasing Saturated Fatty Acid Content<sup>32</sup>**

Table 2 presents the general impacts of the fatty acids presented in Figure 1. Saturated fatty acids have higher CN, cloud point, and stability than monounsaturated and polyunsaturated acids. Thus, diesel made from canola oil, which contains a very high proportion of monounsaturated fatty acid, as shown in Figure 1, has a medium to low CN, cloud point, and stability. On the other hand, diesel made from coconut oil has a high CN, cloud point and stability. The fatty acid compositions of feedstock oils determine not only the properties of the fuel but also its emission levels and characteristics.

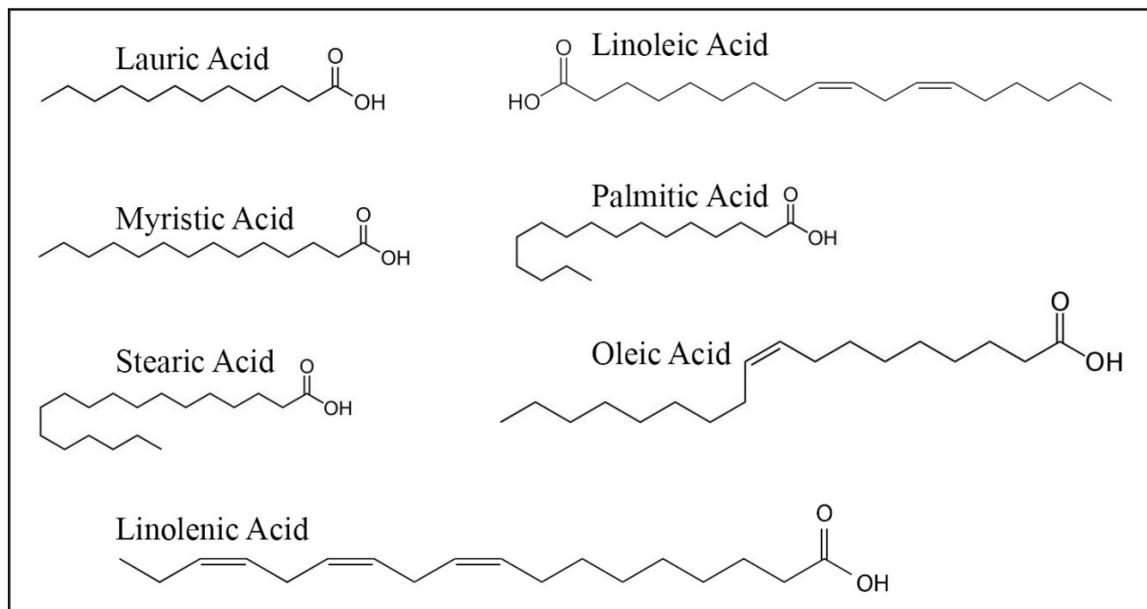
**Table 2. Diesel Fuel Properties as a Function of Composition<sup>32</sup>**

Properties	Saturated	Monounsaturated	Polyunsaturated
CN	High	Medium	Low
Cloud Point	High	Medium	Low
Stability	High	Medium	Low

Other chemical components besides fatty acids also have different concentrations in biodiesel, depending on the type of feedstock and blends. As mentioned above, these differences result in various physical and chemical characteristics and emission components. Therefore, combustion engines that use biodiesel fuels must be designed and operated accordingly to maximize engine efficiency and minimize emissions.

## MODELING STUDY

In the United States, biodiesel is often derived from SME. Figure 2 shows seven molecules commonly found in the biodiesels manufactured using SME and rapeseed oil.<sup>34,35</sup> The most noteworthy common denominator in the structure of biodiesel molecules is the presence of oxygen in the seven common chains (Figure 2). High oxygen content improves combustion efficiency. The fatty acids found in biodiesel fuels and their compositions are summarized in Figure 2 and Table 3, respectively.



**Figure 2. Seven Fatty Acid Molecules Commonly Found in Biodiesel<sup>34,35</sup>**

**Table 3. Typical Fatty Acid Composition-Common Oil Source<sup>34,35</sup>**

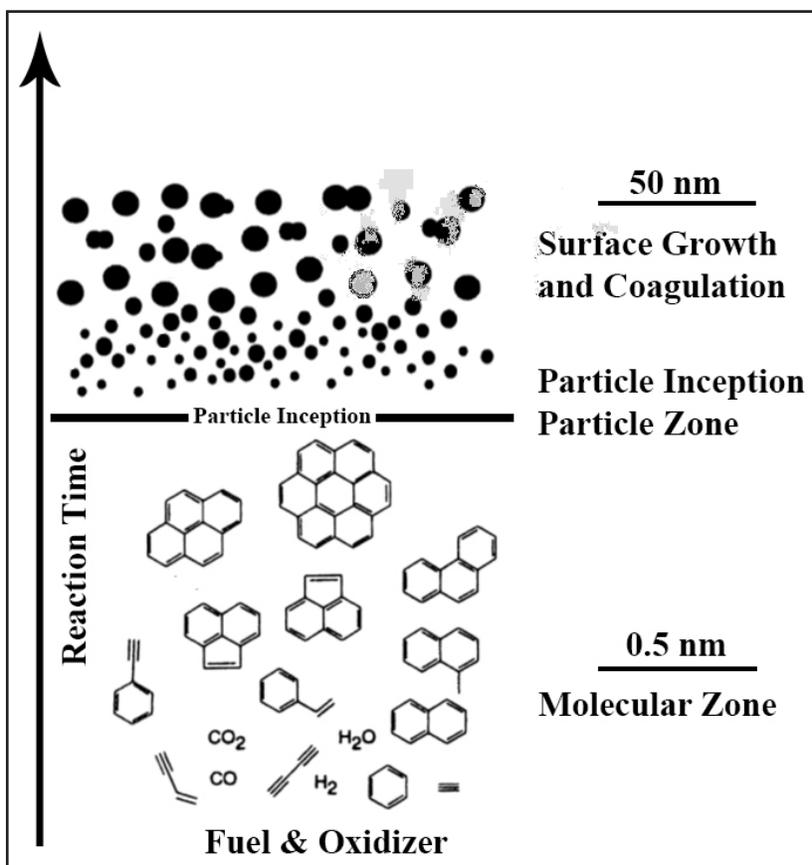
Fatty acid	Soybean	Cottonseed	Palm	Lard	Tallow	Coconut	Rapeseed
Lauric	0.1	0.1	0.1	0.1	0.1	46.5	0.0
Myristic	0.1	0.7	1.0	1.4	2.8	19.2	0.0
Palmitic	10.2	20.1	42.8	23.6	23.3	9.8	4.3
Stearic	3.7	2.6	4.5	14.2	19.4	3.0	1.3
Oleic	22.8	19.2	40.5	44.2	42.4	6.9	59.9
Linoleic	53.7	55.2	10.1	10.7	2.9	2.2	21.1
Linolenic	8.6	0.6	0.2	0.4	0.9	0.0	13.2

As shown in Figure 2 and Table 3, and also as stated above, the chemical structure and composition of biodiesel may vary depending on its feedstock, and this variation may cause significant variations in combustion chemistry and emission compositions. Likewise, various biodiesel contents in different blends may result in different exhaust compositions. Furthermore, variations of chemical structure and vol% of biodiesel may affect the combustion temperature and pressure. Due to the complexity of the biodiesel structure and wide variety of the biofuel structures reported in real-world studies, efforts have focused

on the development of mechanisms for surrogates (alkyl esters). A few studies have been done on kinetics of methyl esters. Most of these have focused on methyl butanoate (MB).

Combustion devices in real-world conditions sometimes deviate from ideality and if the oxygen is not sufficient to burn fuel according to the stoichiometric equation, products of incomplete combustion, such as CO, HCs, and soot, appear beside water and carbon dioxide (CO<sub>2</sub>). Soot is the carbonaceous particulates formed during incomplete gas phase combustion, where the solid phase exhibits no unique physical/chemical structure. Soot formation from engines is of great concern due to its development into PM and its health and environmental impacts on humans. A possible explanation of the hazardous health effects of soot is its association with polycyclic aromatic hydrocarbon (PAH), which has been found to be mutagenic or tumorigenic.

It is obvious that the formation of soot, i.e., the conversion of a HC fuel molecule containing few carbon atoms into carbonaceous agglomerate containing some millions of carbon atoms, is an extremely complicated process, and details of soot formation are still under investigation. However, there is considerable agreement on the general characteristics of the processes involved in soot formation. The characteristic processes of soot formation are depicted in Figure 3.



**Figure 3. A Conceptual Picture of the General Agreement on Soot Formation in Premixed Flames<sup>36</sup>**

Figure 3 shows that fuel is degraded during oxidation into small HC radicals, as shown in the bottom of the figure. HC radicals combine to form aromatic rings that contain a sufficiently large number of carbon atoms. Larger aromatic rings are formed mainly by the addition of acetylene. Primary soot particles are supposed to form by coagulation of larger aromatic structures. Detailed formation mechanisms of soot remain poorly understood, but there is considerable agreement on the general processes, which are summarized as follows:<sup>37</sup>

- Formation of soot precursors
- Nucleation or inception of particles from heavy PAH molecules
- Mass growth of particles by addition of gas phase molecules
- Coagulation via reactive particle-particle collisions
- Oxidation of PAHs and soot particles

### **Formation of Soot Precursors**

Soot precursor molecules are thought to be heavy PAHs that have 500 to 1000 amu. Much attention has been given to the growth process of PAHs by the addition of C<sub>2</sub> and/or C<sub>3</sub> (particularly acetylene). Comprehensive reviews and literature regarding soot formation are available elsewhere.<sup>38</sup>

### **Nucleation or Inception of Particles from Heavy PAH Molecules**

Nucleation bridges the transition from gaseous media in a combustion process to heavy molecules that eventually turn into soot. The molecular mass is approximately 2000 amu,<sup>39</sup> but it is commonly believed that nucleation starts at 300–700 amu.<sup>40</sup> Chemical details of the formation of nascent soot particles are relatively poorly understood, mostly because of experimental difficulties. Several theories, based on the type of molecular precursors, have been proposed in the literature.<sup>41,42</sup>

### **Mass Growth of Particles by Addition of Gas Phase Molecules**

The mechanism for soot surface growth is not well understood. Freenklach<sup>39,40,43</sup> introduced the surface growth reaction mechanism back in the 1980s. The mass of nascent soot particles is increased via the addition of gas phase species (acetylene and PAH). The reaction-radical sites on soot particles are involved in the mass growth process. Mass growth also occurs in low temperatures, even below the lower limit required for the homogeneous nucleation of soot particles.

### **Coagulation via Reactive Particle-Particle Collisions**

During nucleation, particles grow either by coagulation (the combination of two or more particles to form a larger particle, which is efficient for large numbers of particles) or by

condensation (condensation of gas or vapor molecules on the surface of existing particles, which is efficient for large surface areas). Sticking collisions between particles during the mass growth process significantly increase particle size and decrease the number of particles without changing the total mass of soot present. The particle coagulation process occurs almost immediately after soot particle formation or at the beginning of soot formation.<sup>44,45</sup>

## Oxidation of PAHs and Soot Particles

Oxidation takes place on the surfaces of soot particles and decreases the mass of PAHs and soot due to formation of CO and CO<sub>2</sub>. Unlike the surface growth of soot, which occurs in a specific step, oxidation takes place continuously during soot formation. The soot oxidation reduces the carbon mass accumulated in the soot particles.<sup>4</sup> Oxidant elements under fuel-rich conditions are oxygen radical, O<sub>2</sub>, and OH, but in fuel-lean media O<sub>2</sub> while H<sub>2</sub>O, CO<sub>2</sub>, NO, N<sub>2</sub>O, and NO<sub>2</sub> are also possible oxidants.<sup>46,47</sup>

## OBJECTIVES

Vehicles operate at varying loads (due, for example, to traffic congestion, loading weight on board, slope of the road, etc.), and at times when engines remain idle for long durations. As both the load on engine and engine idling make significant contributions to total exhaust emissions, United States Department of Transportation (USDOT) has identified the reduction or elimination of engine idling of public transit buses as a potential component of future state implementation plans. Although the total number of the transit bus engines may be small when compared with other vehicle engines, their emissions counted as a significant source of total diesel PM in urban areas.<sup>4</sup>

To reduce emissions from vehicles, USEPA<sup>1</sup> has advised that an engine should be shut off if idle mode takes more than a few minutes because typical heavy-duty buses can burn approximately one gallon of diesel fuel for an hour in idle mode. Newer vehicles are designed to start easily at all temperatures without idling. Retrofits and cleaner fuels in combination with pollution control equipment, such as PM filters, can also reduce PM emissions. Table 4 presents the USEPA standards for new trucks and buses.<sup>1</sup> The USEPA standards for truck and bus PM emissions standard was reduced by a factor of 10 between 2004 and 2007-2011.

**Table 4. USEPA Standards for New Trucks and Buses<sup>1,a</sup>**

Year	1984	1988	1990	1991	1994	1998	2004	2007-2011
PM emissions <sup>b</sup>	0.6	0.6	0.6	0.25	0.1	0.1	0.1	0.01

Notes:

<sup>a</sup> Urban transit buses have had more stringent standards since 1993.

<sup>b</sup> USEPA's emission standards for trucks and buses are based on the amount of pollution emitted per unit of energy (expressed in grams per brake horsepower hour).

In our laboratory, different types of biodiesel and biodiesel blends were tested using a specific laboratory setup to determine the emission gases produced under various combustion conditions. Additionally, physical properties of different blends and feedstocks (cloud point,

kinematic viscosity, and flash point) were also measured. The resulting data were used to investigate the combustion mechanisms and emission formation mechanisms, as well as to correlate them with the field data. The analyses of the biodiesel emissions provided important information for determining statistical and chemical reaction parameters for combustion modeling.

The purpose of the current study can be stated as follows:

1. To develop a database of pressure-temperature combustion characteristics of biodiesels of different blends and types
2. To model biodiesel combustion based on major HCs under simplified combustion conditions
3. To determine the optimum conditions for minimizing emissions while maximizing combustion efficiency
4. To study physical and chemical characterization of contaminants released during combustion when different biodiesel feedstocks and blends are used

This study was performed to gain a better understanding of the interaction between the above-stated parameters (feedstock, blend, temperature and pressure) and exhaust emissions by characterizing PM from a variety of emission-source categories. Analytical data of biodiesel in this study may be used for new engine design, engine modification, and optimization. The engine efficiency and emission data will be helpful in establishing environmental standards and regulations for biodiesel manufacturers, engine designers, manufacturers, and consumers.



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## II. LITERATURE REVIEW

The literature review is divided into four sections: biodiesel physical properties, laboratory experiments and process conditions, PM characterization collected from field experiments, and modeling.

### BIODIESEL PHYSICAL PROPERTY

Over the past few decades, fossil-fuel energy consumption has increased at a precipitous pace.<sup>48</sup> To maintain the balance between supply and demand of energy, interest in alternative energy has increased.<sup>49-51</sup> Biodiesel is one of the most readily available renewable sources that can be used without much modification of the current infrastructure.<sup>52</sup> It has become more attractive recently because of its superior environmental benefits over conventional fuels and also because of its sustainability.<sup>49,51</sup> Its feedstocks are carbon neutral and have low sulfur content, which greatly assists in the mitigation of environmental effects, such as global warming and air pollution.<sup>52</sup> Biodiesel, a natural and renewable fuel, is generated from vegetable oil, animal fat, grease, WCO, and many other oils with the same nature, through transesterification process, a method which is widely used.<sup>49-53</sup> Based on its similar features as petroleum fuels, biodiesel was put to use in vehicles. Therefore, it is very important to know the essential properties of the different biodiesels. To completely replace or to use biodiesel to meet a major portion of transportation energy needs, more in-depth study on its physical properties is needed. The properties which play a vital role in deciding the biodiesel blend, addition of additives into the fuel, engine functioning, vehicle survival in harsh climates are cloud point, pour point, kinematic viscosity, CN, flash point, ash content, sulfur content, carbon residue, acid value, copper corrosion and higher heating value.<sup>50,51,54</sup> Each and every property of the biodiesel has its own range of importance and not all the properties lead to the same kind of effect on the engine performance and environment. Because our main objective of the study is about PM emissions from buses, we focused on kinematic viscosity, cloud point and flash point of various biodiesel and their blends. Failure in meeting the required ASTM standards set for biodiesel, especially in the case of these three properties, may directly and indirectly affect the amount of PM release.

### LABORATORY EXPERIMENTS

Due to the complexity of biodiesel structure, very few experimental data on different feedstocks and blends of biodiesel are available for the validation of kinetic modeling and/or engine modeling. A large portion of the experimental studies focused on biodiesel combustion in diesel engines, and the results on fuel characteristics and engine conditions were reported.<sup>55-59</sup>

A good knowledge of the kinetics of biodiesel combustion is required to predict combustion performance and emission characteristics of fuel and engines. One of the previous studies on biodiesel combustion was about rapeseed methyl ester (RME) combustion for the first time in a jet-stirrer reactor by Dagaut et al.<sup>55</sup> In another study, Hakka et al.<sup>60</sup> examined the stoichiometric oxidation of two blend surrogates for diesel and biodiesel fuels in a jet-stirred reactor over a wide range of temperatures (550–1100 K). Their experimental results<sup>60</sup> have been compared in order to highlight similarities and differences in the oxidation of large

methyl esters and normal alkanes. None of these studies have reported much information on emissions and the effect of key parameters on emissions. Omidvarborna et al.<sup>61</sup> combusted SME blends with ULSD and SME in a closed chamber at two different temperatures and pressures to analyze CO, CO<sub>2</sub>, CH<sub>4</sub> emissions, and elements of PM. SME with blends of B05 (5% biodiesel, 95% regular diesel), and B20 and ULSD were combusted in a closed chamber at 500, 550 °F and 300, 350 psi. Elemental analyses of collected PM were performed and the results were discussed. This study was unique and valuable because very few studies were done on the effects of combustion conditions on exhaust emissions with different biodiesel feedstocks and blends.

## FIELD EXPERIMENTS

As most biodiesel studies have focused on engine performance and modeling, experimental data on PM emissions from transient buses fueled with biodiesel blends such as B20 are relatively limited in the literature. A very few sources are available that describe a baseline for PM emissions from idling, and furthermore the detailed characteristics of PM produced under various engine conditions have not been investigated either.<sup>62</sup> PM characterization needs a large number of updated analyses due to the continual advances in engine technology and fuel specifications. Therefore, it is thought to be very helpful to understand detailed characteristics of PM with actual operating conditions and fuel specifications. Fuel combustion and its resulting emissions are affected by engine type, size, model, fuel type, post-exhaustion treatment processes, and other parameters, such as fuel additives and catalytic converters. To characterize PM and to find the relationship between emissions and fuel characteristics, we have investigated all major constituents under minimum loads (less than 10 percent).

There are many studies on light-duty engine emissions that reported a decrease in PM with an increase in biodiesel content in fuel. These studies discussed biodiesel emissions from medium and heavy-duty engines. Wang et al.<sup>63</sup> compared the exhaust emissions from in-use heavy trucks fueled with a biodiesel blend of B20 with the emission from B35. The test results showed that the trucks with B35 emitted significantly less PM by about 25%. The main reason for the PM reduction is thought to be the higher oxygenated content of biodiesel over regular diesel. In addition to the higher oxygen content of biodiesel, a reduction in localized fuel-rich regions was observed in the presence of biodiesel, and it was considered a contributing factor in PM reduction. Delocalization of fuel-rich regions in an engine is another factor that reduces soot formation. Reyes and Sepúlveda tested blends of diesel-crude biodiesel and diesel-refined biodiesel in a diesel engine to measure the PM emission.<sup>64</sup> The result showed nearly 50% reduction in PM with respect to the regular diesel when 100% refined biodiesel was used. The chemical and toxicological characteristics of PM emissions from an urban bus engine fueled with diesel and biodiesel blends were studied by Turrio-Baldassarri et al.<sup>65</sup> The experimental study by Canakci<sup>66</sup> comparing biodiesel with ULSD showed that biodiesel achieved a significant reduction in PM. Controversial though it may be, the variety of PM reduction results by switching from conventional fuel to biodiesel produced from various feedstocks have been established proven in various literature.<sup>67-69</sup>

On the other hand, some researchers presented that using biodiesel or its blends increased PM formation when engine vehicles were tested. For example, Mazzoleni et al.<sup>70</sup> examined fleets of school buses to evaluate the effects of biodiesel on exhaust and PM emissions. Interestingly, PM emissions from the school buses significantly increased (up to a factor of 1.8) after the switch from petroleum diesel to B20.

EC and OC are particulate aerosols formed from incomplete combustion. The ratio of OC to EC varies by fuel types, combustion efficiency, and the extent of emissions control. When fossil fuels burn, EC tends to be formed in much higher concentration than OC. Generally, EC is thought to have both a direct warming effect, by absorbing incoming solar radiation in the atmosphere, and an additional warming effect by reducing the albedo (reflectivity) of snow and ice. OC is generally thought to have a direct cooling effect by reflecting the incoming sunlight.

A review of the literature indicated that studies on EC and OC from both hot and cold idling were rare. Similar variation trends of EC and OC were observed in previous studies in running mode.<sup>71-73</sup> The literature study showed that little research has been conducted on OC and EC in PM emissions from biodiesel in hot/cold idle modes. Some OC/EC experiments on diesel engine fueled with biodiesel blends have been done in the past.<sup>26,72-74</sup> They reported that EC emissions decreased with an increasing proportion of biodiesel.

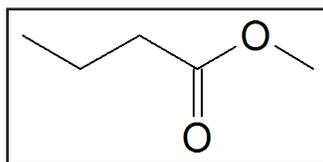
Three light-duty vehicles in five different configurations were tested by Cheung et al.<sup>73</sup> using a dynamometer to develop an improved understanding of the factors affecting the toxicity of PM in exhaust emissions from biodiesel blends. Interestingly, they observed that biodiesel in light-duty vehicles led to an increase in OC emissions and a decrease in EC emissions of 70-85% in several driving cycles. Diesel fuel with a nominal sulfur content of 50 ppm (or 0.005% wt) was used in their study. Finally, Cheung et al.<sup>73</sup> concluded that B20 blend was more efficient than B100 as the increase in OC was very low while the decrease in EC was half of what can be obtained using B100. The EC production during combustion could be disrupted by the oxygen in biodiesel ester atoms. The study of Lu et al.<sup>72</sup> was focused on size distribution of EC and OC from a direct-injection diesel engine fueled with three different fuels.

The carbon speciation of exhaust PM from public transit buses running on both ULSD and B20 was evaluated by Shandilya and Kumar.<sup>71</sup> They studied PM, which was collected on quartz filter papers for both EC and OC. They observed a 6.86% increase in OC and 36.11% decrease in EC when changing from ULSD to biodiesel, respectively. The average OC/EC ratio was 9.82 and 5.66 for biodiesel and ULSD, respectively.

Reduction of PM in exhaust emissions achieved by switching to biodiesel blends highlighted the fact that PM from exhausts can be controlled by biodiesel. PM reduction also accompanies the reduction of elements, and it is important to know what sources cause an increase or decrease of elements in an engine. Inside an engine, fuel and fuel additives including lubricants and antioxidants, and engine parts are present under high temperature and varying pressure, and therefore the chemical composition and the toxicity potential of the exhaust PM might be changed depending on these factors.

## MODELING

Biodiesel mainly derived from soybean oil in the US is comprised primarily of complex structures as depicted in Figure 2. A few studies have been done on kinetics of methyl esters, and most of these studies have been focused on MB. MB (as shown in Figure 4) is a relatively simple methyl ester that possesses the primary features of biodiesel. Also, the MB molecule was considered large enough to allow fast isomerization reactions, which are important in low-temperature combustion chemistry.<sup>75-77</sup> The first detailed chemical kinetic of MB was presented in 2000 by Fisher et al.<sup>77</sup> and it has been tested against the limited experimental data. Since then, the mechanism has been revised by other researchers as well.<sup>56,78-80</sup> MB is a very simple surrogate for biodiesel combustion study which has consistency with experimental data.<sup>79,81-83</sup>



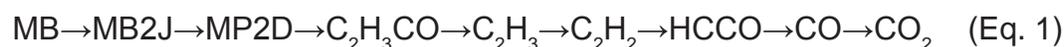
**Figure 4. The Structure of MB (Simple Surrogate of Biodiesel)**

Few models were proposed for detail biodiesel combustion and one of them is Fisher's model,<sup>77</sup> which uses 279 species and around 1,259 reactions. Since Fisher's study, many models were proposed, but the most complete kinetic model was presented by Westbrook et al.<sup>84</sup> They reported a very detailed kinetic scheme for the five major components of SME biodiesel and rapeseed biodiesel which contain more than 4,800 chemical species and nearly 20,000 elementary chemical reactions. The large numbers of reactions and species were due to a lack of symmetry in methyl ester molecules and numerous types of side reactions taken into account.<sup>85</sup> In another study, an equal volumetric ratio of n-heptane ( $C_7H_{16}$ ), MB, and Phenyl Methyl Ether (PME,  $C_7H_8O$ ) was assumed to generate biodiesel surrogates by Golovitchev and Yang.<sup>86</sup>

Progress in the knowledge of MB needs two basic components, experimental data and modification of key reaction rates.<sup>35</sup> Therefore, the future development of methyl ester combustion would require both improvements of kinetic mechanisms as well as an expanded amount of experimental data for validation. Numerous chemical reaction mechanisms consisting of thousands of species and reactions have been developed to make accurate predictions of processes involving complex reaction pathways. The reaction mechanisms may continue to increase in size as the kinetic models are still under investigation and being developed.<sup>34,77,87-89</sup> To explain the method used in this study, a few of the previous modeling studies are briefly described here. Brakora et al.<sup>90</sup> reduced the kinetic model of MB made at Lawrence Livermore National Laboratory (LLNL), which has 264 species and 1,219 reactions to a kind of simple mechanism (combined MB/n-heptane mechanism called ERC-mb) with only 41 species and 150 reactions. The simplified model gives predictions in excellent agreement with those of the comprehensive mechanism (good agreement for ignition delay timing). A combined mechanism was applied to KIVA/CHEMKIN engine simulation programs and compared to biodiesel-fueled engine experiments.

Ng et al.<sup>91</sup> simplified Brakora's model from 41 species and 150 reactions into 33 species and 105 reactions. A combination of methods, including peak molar concentration analysis, reaction flux analysis and the removal of individual species were used to develop this model.

Golovitchev and Yang<sup>86</sup> mentioned that their proposed mechanism could be reduced to 88 species participating in 363 reactions. In this approach, the authors quantify the element transformation flux between species to determine a metric that accurately captures the production and consumption of species. The proposed approach was illustrated with highly complex kinetic mechanisms describing oxidation biodiesel surrogate (MB). A scaled simple characteristic pathway of MB combustion that covers close to half percent of MB combustion is presented here:



The simple pathway presented by He et al.<sup>92</sup> which covers part of Brakora's simple pathway<sup>93</sup> is the main branch of other studies that contain a big portion of MB combustion.

As stated above, these models have included many intermediate chemical species and their interactions, and as a result, they cannot avoid a significant complexity of reaction scheme and ambiguity in many combustion schemes. Therefore, because of the complexity of the reaction, the study is focused on final products in combustion systems (e.g. CO<sub>2</sub>, CO, and PM), rather than encompassing the entire combustion scheme. The main reaction pathways which result in final products of our interest were determined and incorporated in modeling.<sup>92,93</sup>

In a traditional soot model, a two-step approach is used to include two competing reactions of soot formation and soot oxidation. Mechanisms that describe fuel decomposition and oxidation have been developed for many HCs in the past few decades and detailed mechanisms have been proposed to describe soot formation. Soot formation is assumed to be directly related to a characteristic pyrolysis product of acetylene rather than fuel itself. The rate coefficient for soot formation is based on the fundamental assumption that the rate of production of soot primary particles follows the rate of acetylene production. Leung et al.<sup>94</sup> reported the rate expression for soot nucleation which was developed to represent direct formation of soot primary particles from acetylene concentration in mol/cm:<sup>3</sup>

$$\text{Nucleation} = 1.0\text{E}4 \exp[-21100/T] \cdot [\text{C}_2\text{H}_2] \quad (\text{Eq. 2})$$

In another study, a two-step model was used by Um and Park to simulate soot emissions.<sup>95</sup> Soot formation was calculated by using a modified equation proposed in the Hiroyasu model.<sup>96</sup> Here, acetylene was considered a soot precursor. For soot oxidation, the Nagle-Strickland-Constable model<sup>97</sup> was employed. The rate of soot mass change was calculated by subtracting soot oxidation from the soot formation. A few recent studies showed that using detailed PAH species can improve prediction on soot formation.<sup>98,99</sup> The soot formation steps used in the study of Sukumaran et al.<sup>99</sup> proceed in the order of soot inception, soot surface growth, soot coagulation, PAH condensation, soot oxidation by O<sub>2</sub>, and soot oxidation by OH. Acetylene is used as the inception species for soot formation.<sup>41</sup>

Although a unique soot precursor has not been identified yet,<sup>36</sup> acetylene (C<sub>2</sub>H<sub>2</sub>) and some other molecules have been suggested as a primary contributor to soot nucleation and its detailed nucleation kinetic was presented by the reaction:<sup>100</sup>



Many researchers have carried out experiments to evaluate diesel engine emissions for various engine conditions and fuels. Usually, the procedure of measuring engine emissions is laborious and costly. The use of computational techniques has emerged as a feasible alternative way in many cases, particularly to highly complex problems which cannot be easily tested by experimental methods. The computational method that is used in this study is referred as artificial neural networks (ANNs).

ANN is a real-time diagnostic, computational, modeling, control and optimization tool that works based on the properties of biological neural systems. ANNs are capable of learning from any data sources including even nonlinear sources and predict the desired values with high accuracy. ANN can be trained to perform a particular function by adjusting the values of the connection parameters called weights between the adjacent elements. The basic processing element of a neural network is a neuron, a biological neuron, which receives inputs from certain sources, performs a generally nonlinear operation, and presents them as the output. On the other hand, they have the ability to learn the relationship between the input and the output. The network usually consists of an input layer(s), hidden layer(s), and an output layer(s). Different learning algorithms may be used when training the ANNs. A popular learning algorithm is the back-propagation algorithm, which has different variants. Algorithms such as conjugate gradient, quasi-Newton, and Levenberg–Marquardt (LM) use standard numerical optimization techniques. Root-Mean-Squared Error (RMSE), R<sup>2</sup>, is used to represent errors.

In the last two decades, few studies have been conducted to simulate exhaust emissions by implementing ANNs.<sup>101-107</sup> Furthermore, not many studies have focused on hot and cold idle emissions, which are necessary for evaluating the impact of idle conditions on biodiesel emissions. The applicability of ANNs has been investigated for the performance and exhaust emission values of a diesel engine fueled with biodiesels (from SME and yellow grease) and petroleum diesel fuels (fuel No. 1 and No. 2) by Canakci et al.<sup>103</sup> The average molecular weight, net heat of combustion, specific gravity, kinematic viscosity, C/H ratio and CN of each fuel were used as the input, while outputs were the brake specific fuel-consumption, exhaust temperature, and exhaust emissions. The back-propagation learning algorithm with three different variants, single layer, and logistic sigmoid transfer function were used in the network. The network has yielded R<sup>2</sup> values of 0.99 and the mean percent errors were smaller than 4.2 for the training data, while the R<sup>2</sup> values are about 0.99 and the mean percent errors were smaller than 5.5 for the test data.

Later on, the prediction of the engine performance and exhaust emissions was carried out by the same authors<sup>105</sup> for five different neural networks to define how the inputs affect the outputs using the biodiesel blends produced from waste frying oil. It was reported that the fifth network was sufficient for all the outputs (the values of flow rates, maximum injection pressure, emissions, engine load, maximum cylinder gas pressure, and thermal efficiency)

while fuel properties, engine speed, and environmental conditions were taken as the input. For all the networks, the learning algorithm, back-propagation, was applied for a single hidden layer. Scaled conjugate gradient (SCG) and LM have been used for the variants of the algorithm. The fifth network has produced  $R^2$  values of 0.99, and the mean percent errors are smaller than five except for some emissions.<sup>105</sup>

In this study, ANN was used with the input data on engine speed, temperature, and manifold intake pressure collected in field experiments to predict PM concentration.



### III. METHODOLOGY

To better understand the research procedure, the methodology is divided into three sections: laboratory experiments, field tests, and modeling approach. It is worth mentioning that all the instruments, especially both gas chromatography and Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) were calibrated with proper standard gas and solution prior to any tests. To reduce the uncertainty in the concentration values in samplings, the analyses were always carried out in the blank samples.

#### LABORATORY EXPERIMENTS

##### Biodiesel Property Tests

In this study, different biodiesels and its blends have been analyzed for cloud point, kinematic viscosity, and flash point and the measured properties have been compared with ULSD.

**Cloud Point:** For petroleum products and biodiesel fuels, cloud point refers to the lowest temperature below which wax in diesel, or biowax in biodiesels, form a cloudy appearance. According to ASTM D2500 cloud point is defined as the temperature of a liquid sample when the smallest observable cluster of wax crystals first appears upon cooling under prescribed test conditions.<sup>108</sup> Below a cloud point, fuel tends to solidify and form crystals, which restrains the movement of engine parts and alters its working efficiency.<sup>50</sup> We followed the ASTM D2500 procedure to measure the cloud point.<sup>108</sup>

**Kinematic Viscosity:** In a vehicle, petroleum and non-petroleum products are used as lubricants depending on the viscosity of the fuel being used. The viscosity of the fuel is important for handling and storage.<sup>109</sup> Viscosity of the vegetable oils is 9 to 17 times greater than the petroleum diesel fuel.<sup>110</sup> Kinematic viscosity is the coefficient of viscosity of a fluid divided by its density, usually measured in centistokes (cSt).<sup>109</sup> ASTM D445 standards were followed for this test.

**Flash Point:** Flash point measures the specimen's tendency to form a flammable mixture with air under controlled laboratory conditions.<sup>111</sup> It is only one of several properties that should be considered in estimating the overall flammability hazard of a material.<sup>111,112</sup> An abnormal flash point can be associated with contamination of the material.<sup>111</sup> ASTM D92 Cleveland open cup test standards have been used.

##### Experimental Setup and Procedure for Property Tests

Cloud point, kinematic viscosity, and flash point tests were conducted on ULSD (i.e., B00), B10, B20, B50, and B100 blends of SME, TO from animal fat and WCO.

For the cloud point test, the most important apparatus is a water bath. A test jar of 32.5 mm diameter and cork with a provision to insert a thermometer was taken. A 40 mm layer of biodiesel was transferred into a test tube. According to the ASTM D2500 standards, different water baths are prepared using sodium chloride (NaCl), calcium chloride (CaCl<sub>2</sub>), dry ice,

water, and ice. The test fuel is placed inside the bath and checked for a cloud point and if it doesn't happen in one bath then another bath in a different temperature range is used and a cloud point temperature is noted.<sup>108</sup> Table 5 shows the bath and sample temperature ranges. The test was repeated 4 times to increase accuracy of the results.

**Table 5. Bath and Sample Temperature Ranges (taken from ASTM D2500-02)**

Bath	Bath Temperature Setting (°C)	Sample Cloud Point Temperature Range(°C)
1	0 ± 1.5	Start to 9
2	-18 ± 1.5	9 to -6
3	-33 ± 1.5	-6 to -24
4	-51 ± 1.5	-24 to -42
5	-69 ± 1.5	-42 to -60

Kinematic viscosity test is an essential part of the tests because viscosity affects the atomization of a fuel upon injection into a combustion chamber and, thereby, the formation of engine deposits. The tendency of the fuel to cause particle deposition is higher as viscosity increases. To perform the kinematic viscosity test, a sample biodiesel, calibrated viscometer, a beaker with a liquid medium inside maintained at 40 °C, a stop watch, a thermometer to measure the liquid medium temperature, a heater and a viscometer holder were needed. ASTM D445 standards were used. The calibrated Cannon-Fenske Routine Viscometer, size 75 was filled with 7 ml of biodiesel and placed inside the beaker for 10 minutes in order to heat the fuel. It was then pulled up and released, so as to calculate the time taken by the biodiesel to pass through the marked circles on the viscometer.<sup>109</sup> This test was repeated four times to increase accuracy of the results.

The Flash Point Test is a significant test that determines the lowest temperature at atmospheric pressure, at which vapors are created due to heating of petroleum products or biodiesel igniting under induced flame.<sup>111</sup> For safety concerns, such as storage, knowing the flash point value of a fuel is imperative.<sup>112</sup> To carry out a flash point test, the Cleveland open test cup, test flame, heating plate, thermometer and holders are needed.<sup>111</sup> The kinematic viscosity experiment was carried out at a room temperature of 21±0.5 °C. 70 ml of a flammable liquid (here biodiesel and ULSD) is taken into the Cleveland open test cup and placed over a heating pan. It is heated at a rate between 5 to 17 °C/min (here 10±1 °C/min was maintained). The rate of temperature increase was reduced to 5 to 6 °C for the last 28 °C before the flash point. The temperature raise was measured using a thermometer, which was placed inside the liquid without touching it to the surface of the cup. A test flame was passed over the liquid to ignite the possibly existing flammable vapor and the temperature at which a blue color flame appeared for less than a second was noted as flash point.<sup>111</sup>

### Experimental Setup for Combustion Tests and Procedure

A 300 ml stainless steel reactor (Model 4766HT-FG-SS-3000, 2.5" inside diameter with 4.0" inside depth) designed by Parr Instrument Company was used to perform the fuel combustion under high-temperature, high-pressure conditions. The highest pressure that

this batch-type reactor can hold is 3000 psi; the highest temperature, 1000 °F, and the upper limits for operating pressure and temperature are 2000 psi and 850 °F, respectively. For safety reasons, two different pressures (300 and 400 psi) were selected at which the combustion temperature never surpassed the maximum operation limit (<1000 °F). A heating assembly with a stand and temperature controller was installed to preserve the reaction conditions at the predetermined values. A noble gas (helium) was used to maintain higher pressure during combustion. The combustion chamber is represented in Figure 5. A schematic diagram and photograph of the entire experimental setup and gas chromatograph are shown in Figure 6 and Figure 7, respectively.

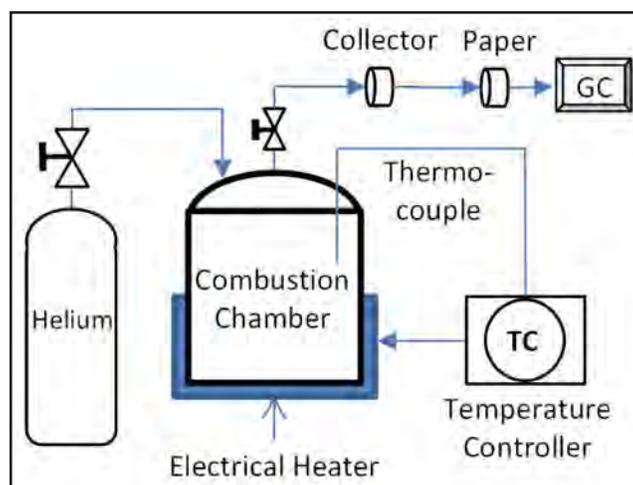


(a)



(b)

**Figure 5. (a) Combustion Chamber with a Pressure Gauge, Thermocouple, Inlet, and Outlet Ports; (b) Heating Unit and Temperature Controller**



**Figure 6. Schematic Diagram of Experimental Setup**



**Figure 7. GC Connected to the Reactor for Analyzing Emission Compositions**

A 4 ml sample of biodiesel or blend was obtained and placed in the chamber. The reactor temperature was monitored by a J-type thermocouple placed at the center of the reactor. With this arrangement, the reaction temperature could be controlled and monitored with a precision of 0.1 °C. The pressure of helium gas was pre-determined depending on the combustion conditions. The test samples are grouped into different types of biodiesel feedstock (SME, TO and WCO) and their blending (B00, B20, B50 and B100). Thus, for every temperature and pressure, the samples to be tested were ULSD (B00) and a volume percentage of biodiesel fuel blended with ULSD, such as SME 20%, 50% and 100%. The same ratio was used for TO and WCO. ULSD was used as a control in combustion experiments. The retention time of the reaction was determined by observing the reaction conditions (T/P) and set points. The upper and lower combustion conditions were set based on system tolerance (upper T/P).

The heater began to increase system temperature to the designed value, close to auto-ignition temperature, and pressure increased rapidly as the temperature increased due to combustion. After auto-ignition occurred, both the temperature and the pressure increased rapidly toward their peak values and remained constant until the combustion was terminated.

After the combustion temperature reached the pre-set temperature, the emission gas was released and allowed to pass through a Teflon (PTFE) filter paper 47 mm in diameter. As the emissions passed through the filter paper, particulate matter greater than 0.5  $\mu\text{m}$  in size was retained on the filter. The filter papers were stored for PM elemental analysis. For the metal analysis of PM, a microwave-accelerated-reaction system (MARS) and ICP-OES were used.

Presence of any blockage in the GC column due to PM compromises the quality of emission gas analysis results. To prevent the blockage, a PTFE membrane filter capsule with 0.2  $\mu\text{m}$  pore size was placed before the GC inlet. The filtered gas was passed through the GC to be analyzed for the concentrations of  $\text{O}_2$ ,  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ , and  $\text{CH}_4$ . A Shimadzu 2010 GC, with a PDHID (pulsed-discharge helium ionization detector), was used for real-time analysis. The type of column used was Carboxene 1010 Porous Layer Open Tubular (PLOT), which has a length of 30 m and an internal diameter of 0.32 mm.

Teflon filter papers were mounted on a smooth Cu-alloy stub for the Environmental Scanning Electron Microscope (ESEM) analysis, and the particles were observed at 10-30 kV with Quanta 200 3D ESEM (FEI/Phillips, Germany) to obtain the morphology, size, and shape of individual particles.

PM could have been deposited on the wall of the reactor (after combustion occurred) or in connecting lines (during sampling). In this study it is assumed that the possibility of PM deposition was the same for all tests, and the PM deposited on the wall and tubing was not included in emission gas analyses.

## FIELD EXPERIMENTS

Two identical sets of TARTA transit buses running on B20 (each set containing five on-road buses) were selected for both the hot and cold idling tests (i.e., the minimum load, acceleration, and speed were zero). (The future regulatory plans of the Federal Transit Administration identified idle mode as a pollution source.) In studying idle mode, a constant volume flow rate could be assumed in the calculations for the exhaust flow rate.<sup>113</sup>

To avoid the influence of existing PM inside the garage, the sampling was conducted outside in an open area. Sampling was done by CatchCan,<sup>71</sup> which was used directly on the tip of exhaust pipe. Due to lack of information on the exhaust flow rates, the results for the 700 series were converted to a concentration format using the Donaldson Engine Exhaust Flow Guide. The exhaust-flow rate data was obtained at a maximum rpm, so it could be easily compared with results from a previous study by the authors.<sup>62</sup> The exact exhaust flow rate was measured by connecting the engine to a computer software program called "Energy Service Insite," provided by Cummin, Inc. Table 6 summarizes the main engine parameters for the three different series.

**Table 6. Specification of Tested Transit Buses (Main Engine Parameters)**

	Bus Series		
	50069	700	800
Engine	MBE900 Mercedes Benz	Cummins ISL6LTAA	Cummins ISL-07
Chassis	Thomas	Gillig	Eldorado National
Year of Mfg.	2003	2003	2010
Gross Vehicle weight (lbs)	28,580	39,000	42,760
Engine Capacity	7.2L	8.9L	8.9L
Maximum Power	260HP	289HP @ 2000 RPM	280HP @ 2200 RPM
Maximum Torque	800 ftlbs@1200rpm	900 ftlbs @1300 RPM	900 ftlbs@1300 RPM
Emission Certifications	2007	2007	2007
Maximum Torque	800 ftlbs@1200rpm	900 ftlbs @1300 RPM	900 ftlbs@1300 RPM

The collection time for PM was 15 minutes, which is similar to previous studies.<sup>114-116</sup> Because of the high exhaust temperature and the collection method, which directly captures PM at the tip of the exhaust pipe, effects of ambient temperature and humidity were assumed to be negligible. The fuel storage tank at the bus depot was refilled with B20 from a local provider. Detail specification of the fuels is presented in Table 1.

Quartz depth filter papers were used due to their characteristics—binder-free, heat-treated to remove trace organic impurities, high-purity microfibers for collecting diesel particulates, low-metal background—which are specified in NIOSH method for EC from SKC, Inc. The PM masses were determined gravimetrically by subtracting the final value of a quartz filter paper from the initial mass of the sample filter. The pre-treatment and post-treatment steps for the gravimetric mass determinations are as follows: 24 hours (40 CFR recommends 1-80 hours) to equilibrate filters before and after weighing, at a temperature of 20 °C and a relative humidity of 50%. This is because the gravimetric method is highly sensitive to the effects of moisture and/or relative humidity (RH), along with static charge buildup on the filter papers. The gravimetric analysis needs highly precise weighing and an enhanced quality assurance effort to obtain reliable measurements. The higher the sensitivity of the balance, the higher the quality of the results. PM emissions of each transit bus were tested several times to ensure that the results were accurate. A certified Mettler Toledo XP105 microbalance (maximum capacity: 31 g/120 g, accuracy: 0.01 mg/0.1 mg) placed on a vibration-free table was used for weighing the filter papers.

ICP-OES was used at the U.S. Department of Agriculture (USDA) laboratory at the University of Toledo to evaluate elemental composition. The results of elemental analysis were interpreted using the positive matrix factorization (PMF) model (version 3.0 or PMF 3.0). This is a free software program developed by USEPA that helps in identifying and quantifying the relative contributions of various air pollution sources in ambient air quality. PMF has been used extensively as a means of source apportionment.<sup>117-120</sup> For example, PMF was applied to one-hour gaseous and particulate concentrations from a stationary site in southern California.<sup>121</sup> In this study, for the first time, PMF was used to determine the source apportionment for elements of PM that were emitted from transit

buses in hot and cold idle modes. Detailed information on the software operation, input/output files, uncertainty calculation, and other specifications was provided earlier.<sup>122,123</sup>

RTI Laboratories, Inc., in North Carolina carried out EC and OC analyses on PM collected on filter papers using the IMPROVE\_A method. In this method, seven carbon fractions are defined including OC1 – OC4, and EC1 – EC3. The first four fractions—OC1 – OC4—are determined in a helium atmosphere at 140 °C, 280 °C, 480 °C, and 580 °C, respectively. The other three fractions—EC1, EC2, and EC3—are determined in a 2% oxygen and 98% helium atmosphere at 580 °C, 740 °C, and 840 °C, respectively.<sup>71</sup> The other parameters are defined as follows:

Concentration of pyrolyzed carbon by reflectance (PCR): Carbon evolved between the addition of oxygen and the OC/EC split based on reflectance.

Concentration of pyrolyzed carbon by transmittance (PCT): Carbon evolved between the addition of oxygen and the OC/EC split based on transmittance.

Concentration of OC by reflectance (OCR) equivalent to:

$$\sum OC_i + PCR \quad (i = 1 \text{ to } 4)$$

Concentration of OC by transmittance (OCT) equivalent to:

$$\sum OC_i + PCT \quad (i = 1 \text{ to } 4)$$

Concentration of EC by reflectance (ECR) equivalent to:

$$ECR = TC - OCR$$

Concentration of EC by transmittance (ECT) equivalent to:

$$ECT = TC - OCT$$

More details about the method are presented in “Carbon Analysis of PM” (2009),<sup>124</sup> with a standard procedure for the determination of EC/OC/TC in PM.

PM pollution in urban areas arises from different sources and varies in composition, as mentioned previously. Carbonaceous PM is a fundamental parameter to evaluate atmospheric pollution due to engine combustion and can also be considered as a specific index of motor vehicle traffic pollution. Its separation into EC and OC is toxicologically significant and provides valuable information for the formation mechanisms of photochemical pollution. Carbonaceous fraction is a function of EC, OC, and diesel particulate mass (DPM) based on the following equation:<sup>125</sup>

$$\text{Carbonaceous fraction or CF} = (EC + 1.2 * OC) / PM \quad (\text{Eq. 4})$$

## MODELING APPROACH

As stated above, due to the complexity of biodiesel structure and the size of molecules (as shown in Table 3), comprehensive modeling of biodiesel combustion requires large amounts of experimental data and extensive investigation on the detailed combustion mechanisms. For practical reasons, surrogate molecules that match the characteristics of a real biodiesel have been used to simplify the combustion mechanism, required computational time, and cost. Our approach focuses on MB combustion to complete Fisher's reaction model. Almost all other terminating reactions that lead to formation of CO, CO<sub>2</sub>, etc., were considered. Non-reversible and elementary reactions were assumed to be attributable to fundamental reaction kinetics. The mechanisms are presented in Table 7. Table 7, A, B, and E represent Arrhenius parameters used to calculate the rate of reactions. Other specific elements and reactions were added into the system to achieve higher precision and reasonable results for soot formation and growth.

**Table 7. Kinetic of Simplified Mechanism in MB Combustion with Arrhenius Parameters**

	Reaction	A	B	E
1	$mb+o_2=ho_2+mb4j$	3.00E+13	0.00	52800
2	$mb4j+o_2=mb4oo$	4.50E+12	0.00	0
3	$mb4oo=mb4ooh2j$	2.00E+11	0.00	21989
4	$mb4ooh2j=mp2d+ch_2o+oh$	1.03E+20	-1.58	33380
5	$mp2d+ho_2=c_2h_3co+ch_2o+h_2o_2$	8.40E+12	0.00	20440
6	$c_2h_3co=c_2h_3+co$	2.04E+14	-0.40	31500
7	$c_2h_3+o_2=c_2h_2+ho_2$	2.12E-06	6.00	9484
8	$c_2h_3+h=c_2h_2+h_2$	2.00E+13	0.00	2500
9	$c_2h_2+o_2=hcco+oh$	2.00E+08	0.00	30100
10	$c_2h_2+o=hcco+h$	1.43E+07	2.00	1900
11	$hcco+o=h+co+co$	8.00E+13	0.00	0
12	$hcco+o_2=co_2+hco$	2.40E+11	0.00	-854
13	$c_2h_2+oh=ch_2co+h$	2.19E-04	4.50	-1000
14	$ch_2co+h=ch_3+co$	1.10E+13	0.00	3400
15	$ch_2co+oh=hcco+h_2o$	1.00E+13	0.00	2000
16	$c_2h_2+ch_3=c_3h_4-ah$	6.74E+19	-2.08	31590
17	$c_3h_4-a+ho_2=c_3h_3+h_2o_2$	3.00E+13	0.00	14000
18	$c_3h_4-a+o_2=c_3h_3+ho_2$	4.00E+13	0.00	39160
19	$c_3h_4-a+h=c_3h_3+h_2$	2.00E+07	2.00	5000
20	$mp2d+ch_3=c_2h_3co+ch_2o+ch_4$	4.52E-02	3.65	7154
21	$ch_2o+h=hco+h_2$	9.33E+08	1.50	2976
22	$mp2d+oh=c_2h_3co+ch_2o+h_2o$	5.25E+09	0.97	1590
23	$ch_2o+oh=hco+h_2o$	3.43E+09	1.18	-447
24	$hco+ho_2=ch_2o+o_2$	2.97E+10	0.33	-3861

Although a few studies have been conducted to model diesel engine emissions using ANN, not many of them have focused on idle emission data. These studies do not consider all of the important engine parameters, such as engine speed, temperature, manifold intake pressure, etc., which are thought to play important roles in engine emissions. These parameters are considered here in ANN modeling. The input data, such as coolant and fuel temperature, intake manifold temperature and pressure, and engine speed were added as input parameters for the 700 series. For the 800 series, there are more input parameters from the engines, such as diesel oxidation catalyst intake temperature, diesel particulate filter intake/outlet temperature, EGR temperature, engine coolant temperature, engine speed, exhaust flow rate and intake manifold temperature and pressure.



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## IV. RESULTS AND DISCUSSION

### LABORATORY EXPERIMENTS

Several physical/chemical experiments were done on the samples to present comprehensive analyses on the effects of blends and feedstocks. Results are divided into three sections as shown below.

#### Biodiesel Physical Properties

The value of cloud point varied with the feedstock, biodiesel ester composition and the existence of additives.<sup>53,110</sup> Manufacturing companies maintain the cloud point of a particular biodiesel depending on the season and geographical region. The cloud point value in summer can be greater than in any other season. Cloud point value in temperate regions should be lower than that in tropical regions. As biodiesel properties are determined by feedstock type, biodiesel obtained from semi-drying oils like rapeseed or soybean has better cold-flow properties than biodiesel obtained from animal fat, such as beef or pig tallow.<sup>126</sup>

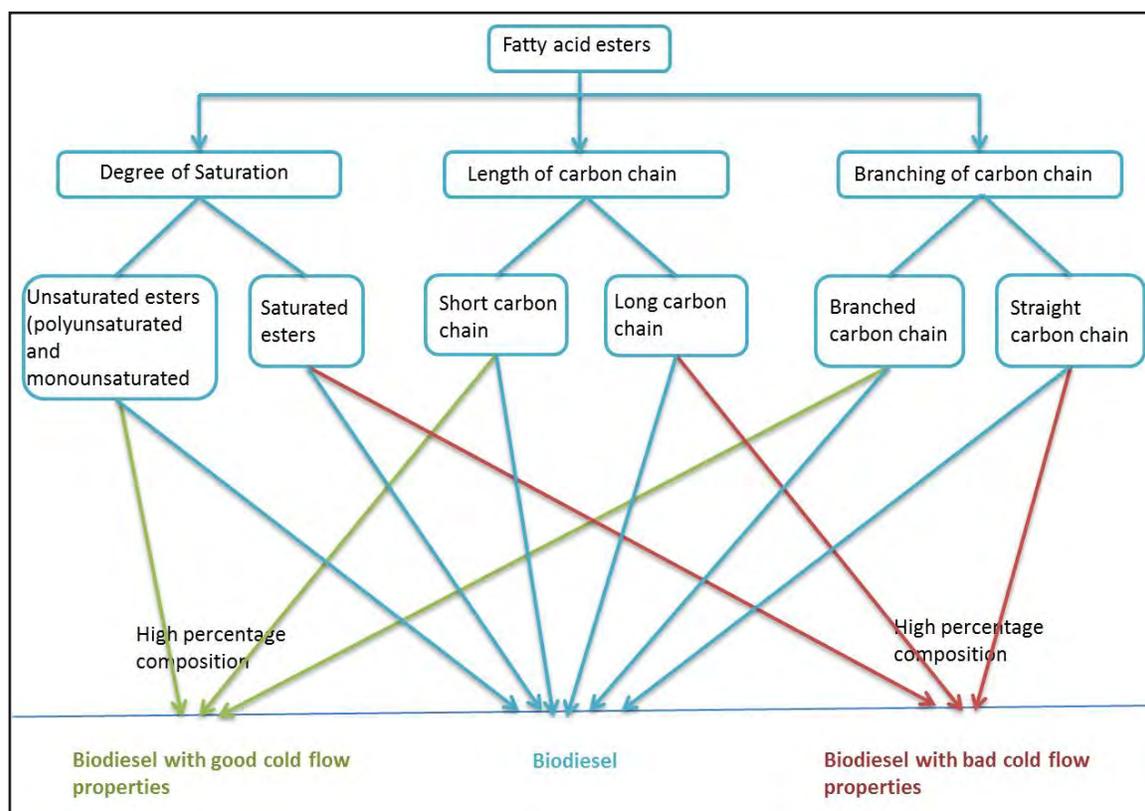
High viscosity is the major problem with most biodiesel feedstocks, such as vegetable, animal fat, and waste oils.<sup>110,127</sup> For this reason, the use of B100 for any biodiesel has been abandoned, and blends were formulated to reduce viscosity.<sup>127</sup> ASTM has proposed a kinematic viscosity range for biodiesel and ULSD fuels that indicates which fuels are safe to use in any motor vehicle and will not clog or inhibit movement of engine parts. The range is 1.9 – 6 cSt for biodiesel and 1.9 – 4.1 cSt for ULSD.<sup>109</sup>

To obtain accurate values and reduce errors, a kinematic viscosity test was conducted multiple times. The precision of the test methods and results was determined using statistical examination of the laboratory results.<sup>108</sup> A standard deviation and linear regression are made to show the variation in cloud point and kinematic viscosity values in terms of blending percentage. Tables 8, 9, and 10 show the results obtained and the standard deviation values for different fuels in cloud point tests, kinematic viscosity tests and flash point tests, respectively. Figures 8, 9, and 10 show the standard deviation of cloud point tests, kinematic viscosity tests, and flash point tests, respectively.

There are no particular ranges set for cloud point of petroleum fuels and biodiesels in the U.S., as climate varies dramatically across regions. Based on the testing results of various authors, SME B100 becomes cloudy at a temperature range from -5 to 2 °C.<sup>50,126,128</sup> In general, feedstocks with a higher percentage of saturated fatty acid have high cloud points and pour point values that can be regarded as undesirable cold flow properties.<sup>32,129</sup> SME has less amounts of saturated fatty acids than TO and WCO.<sup>32</sup> As shown in Figure 9 and in Table 8, the experiment results indicate that the cloud points of 100% SME and its blends B10, B20, and B50 have relatively higher values than TO and WCO, which makes it a biodiesel with better cold-flow properties. TO showed higher cloud points than the remaining two biodiesels and, invariably, its blends also showed high cloud point values.

ULSD, which has a cloud point of -9 °C, is mixed with biodiesel to lower cloud point values. Among the blends, B20 of SME has the lowest cloud point: -7.5 °C with a standard

deviation of  $\pm 0.25$  °C, whereas B50 of TO has the highest cloud point value. Although the cloud point of WCO B20 is -8 °C, it cannot be regarded as a blend with the lowest cloud point because of its higher deviation. Another possible reason for high cloud point values is the existence of longer carbon chains of saturated fatty acids. The longer the carbon chain, the higher the cloud point of the biodiesel.<sup>129,130</sup> Characteristic effects of fatty acid composition on cold flow properties are depicted in Figure 8, which summarizes that the biodiesel with a high percentage of unsaturated fatty acids, branched carbon chain fatty acids and short-chained fatty esters exhibits improved cold flow properties.<sup>129</sup> Branched carbon-chain fatty acids form a structure that needs high thermodynamic force for its crystallization which means biodiesel does not solidify easily, and thus has better cold flow properties.<sup>129,131-133</sup> As shown in Figure 8, this basic relationship of fatty acid structure and biodiesel properties is verified by our results. The relationship may be also used to explain and predict the properties of unknown biodiesel of different blends from various feedstocks. The rationale of this particular section of the report is to test and understand variations of the properties (cloud point, flash point and kinematic viscosity) of biodiesel by blend and type of feedstock.



**Figure 8. Effect of Fatty Acid Composition on Cold Flow Properties<sup>129</sup>**

**Table 8. Cloud Point Temperature of ULSD and Various Biodiesel Blends**

Fuel	Blend	Cloud Point (°C)
ULSD	-	-9.0± 0.50
TO	B100	9.0± 0.48
	B50	0.0± 0.00
	B20	-5.0± 0.41
	B10	-6.5± 0.25
SME	B100	0.0± 0.50
	B50	-4.5± 0.25
	B20	-7.0± 0.29
	B10	-7.5± 0.25
WCO	B100	3.0± 0.25
	B50	-4.5± 0.29
	B20	-6.5± 0.25
	B10	-8.0± 0.71

**Table 9. Kinematic Viscosity Values of ULSD and Biodiesel Blends**

Fuel	Blend	Kinematic Viscosity (cSt), $v=C*t$
ULSD	-	3.44± 0.031
SME	B100	4.91± 0.013
	B50	3.25± 0.026
	B20	2.89± 0.020
	B10	3.38± 0.018
TO	B100	5.63± 0.030
	B50	4.22± 0.013
	B20	3.69± 0.033
	B10	3.43± 0.012
WCO	B100	5.64± 0.022
	B50	4.28± 0.007
	B20	3.70± 0.007
	B10	3.51± 0.021

**Table 10. Flash Point Values of ULSD and Biodiesel Blends**

Fuel	Blend	Flash Point (°C)
ULSD	-	73±0.71
SME	B100	171
	B50	94
	B20	80±0.71
	B10	79

Fuel	Blend	Flash Point (°C)
TO	B100	176±2.21
	B50	106
	B20	89
	B10	84±0.35
WCO	B100	167
	B50	96
	B20	82
	B10	79

Viscosities of methyl or ethyl esters of vegetable oil are nearly twice that of diesel fuels.<sup>134</sup> Table 9 shows that kinematic viscosity of SME is nearly 1.43 times that of ULSD, while TO and WCO are 1.65 times higher than ULSD. Thus, the kinematic viscosity of SME is much better for engine performance when compared to TO and WCO, and this indicates that SME could make fuel with less viscosity when blended with ULSD. The longer the length of the fatty acid saturated methyl esters, the higher the measured viscosity values at 40 °C.<sup>135</sup> More than 95% of soybean fatty acid saturated methyl esters contains palmitic (C16:0), stearic (C18:0), oleic (C18:1), linoleic (C18:2) and linolenic (C18:3) acids. Both WCO and TO contain heavier fatty acids, which result in high specific gravity and kinematic viscosity values.<sup>136</sup> Kinematic viscosities of TO and WCO are approximately equal, even after blending with ULSD.

The flash point of a fuel is an important consideration for hazard management. The minimum value limit of 100% biodiesel (B100) is set at 130 °C and 52 °C for diesel by ASTM standards.<sup>111,137</sup> In the flash point experiments conducted with ULSD, TO, SME and WCO, it was clear that the results were higher than the minimum flash point temperature limit, which is acceptable for engine operation. TO has a high flash point of 176 °C, followed by SME and WCO with 171 °C and 167 °C, respectively. SME and WCO showed similar flash point values. The flash point of biodiesel is affected by triglyceride levels; an increase in triglycerides raises the flash point.<sup>137</sup>

According to the standard deviations shown in Figures 9, 10, and 11 and Tables 8, 9, and 10, the cloud point measurements had minimal variation overall. Kinematic viscosity tests and flash point tests were conducted with high precision except for a small deviation, ±2.21 °C, in TO B100 readings. Kinematic viscosities of ULSD, SME, TO, and WCO were in agreement with the corresponding ranges of ASTM D445 standards. If the kinematic viscosity of the biodiesel was not within standard range, then it was further diluted with ULSD to reduce the viscosity.

Linearity of the results among the blends of different biodiesels was investigated for cloud point. In terms of blends, Figures 12-14 show the linearity trends of SME, TO, and WCO, respectively. Linear line fittings for cloud points of TO, SME and WCO, show linear relations between cloud point and blends.

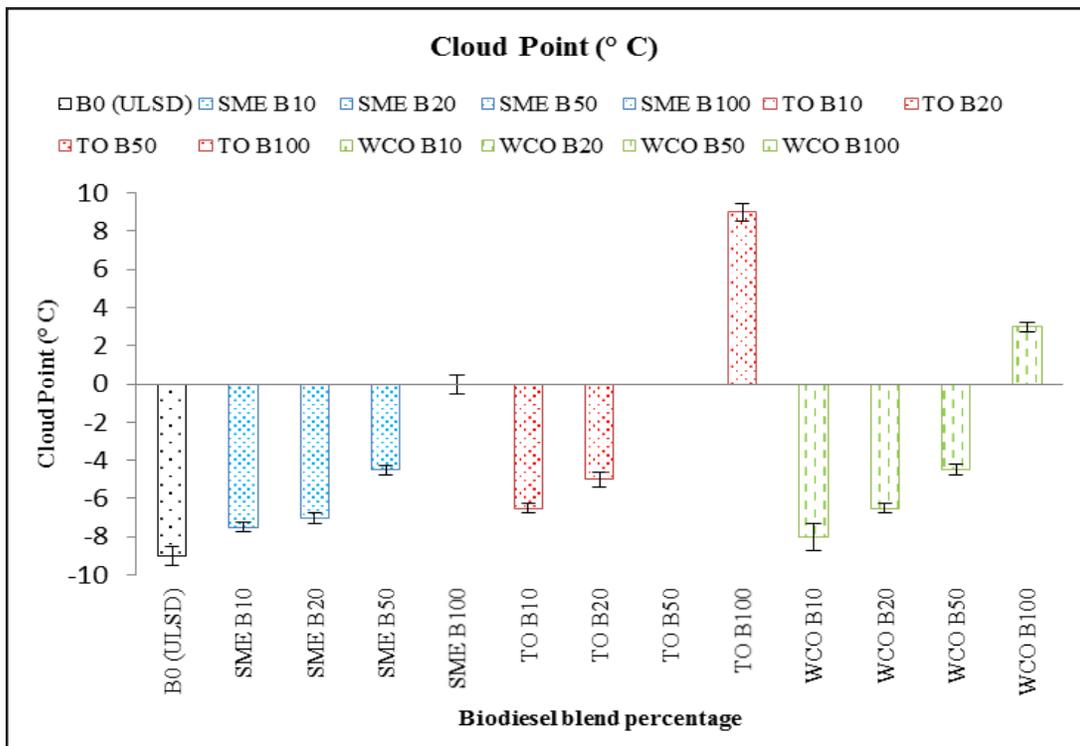


Figure 9. Cloud Point of ULSD and Biodiesel Blends with Standard Deviation

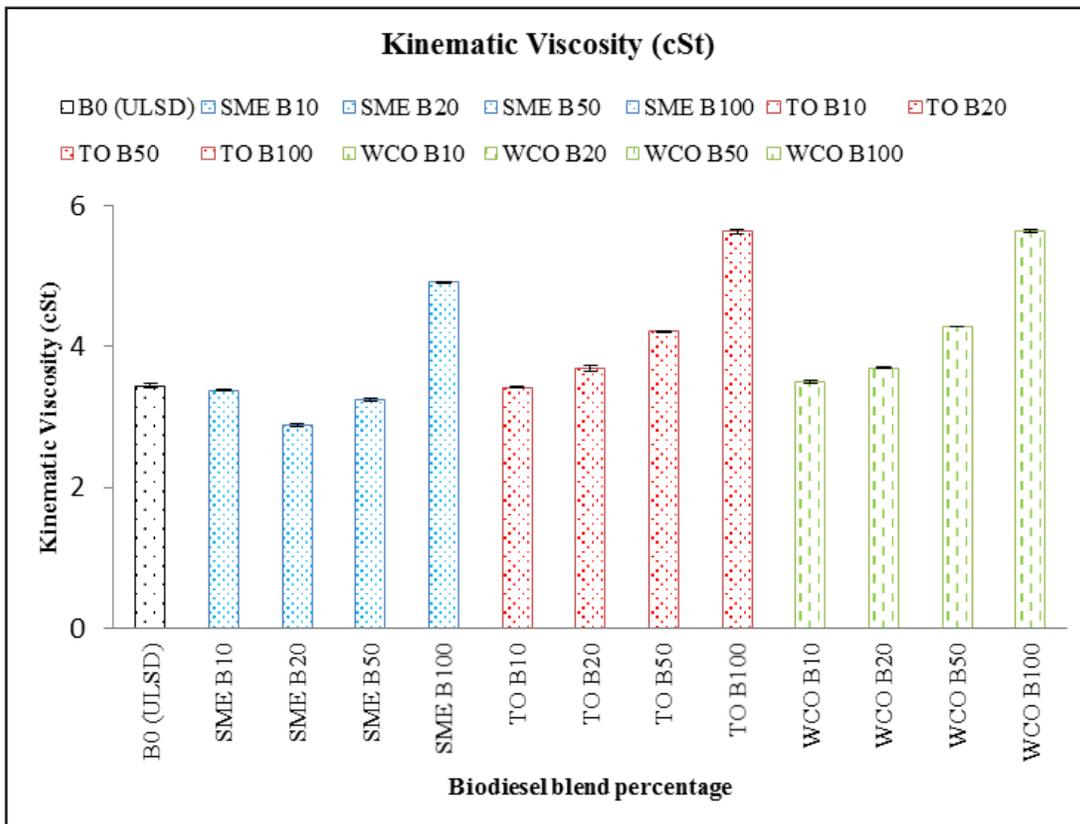


Figure 10. Kinematic Viscosity of ULSD and Biodiesel Blends with Standard Deviation

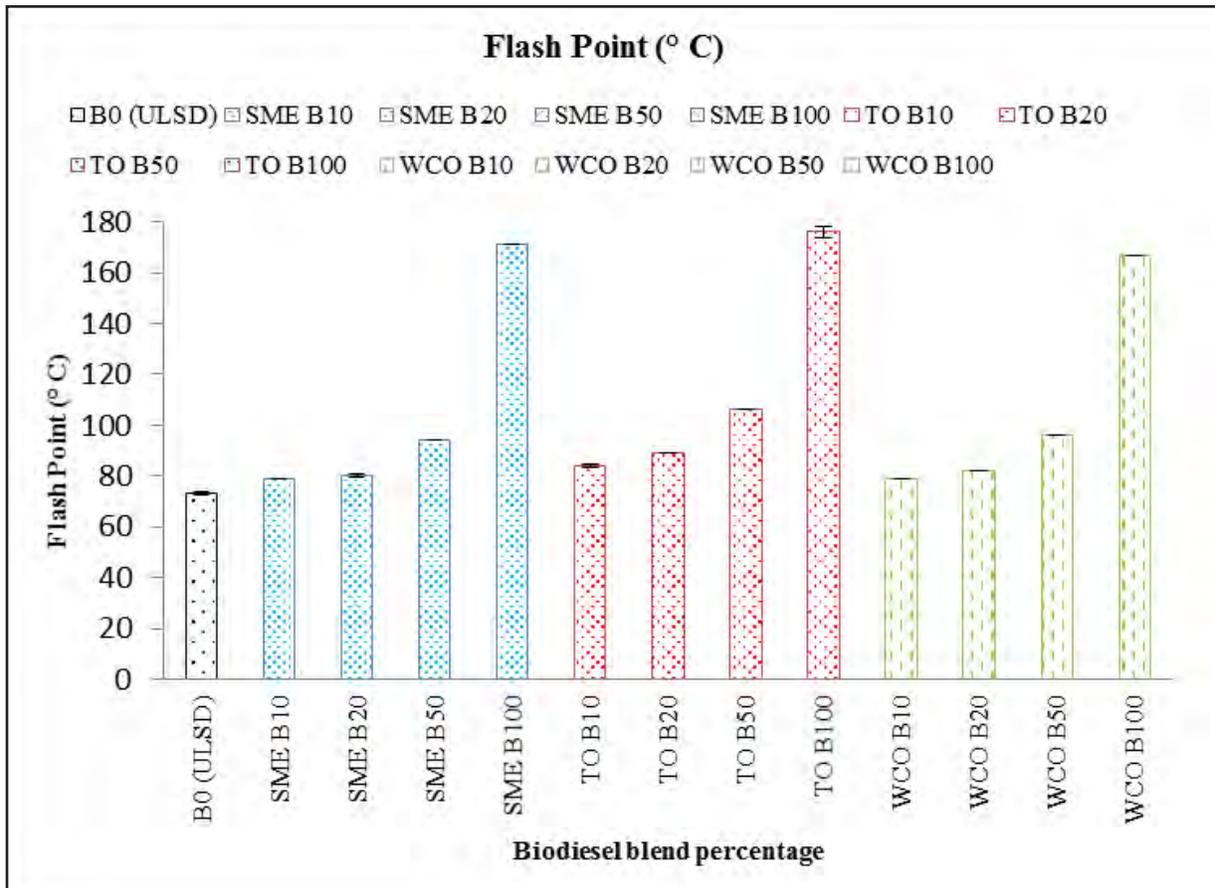


Figure 11. Flash Point of ULSD and Biodiesel Blends with Standard Deviation

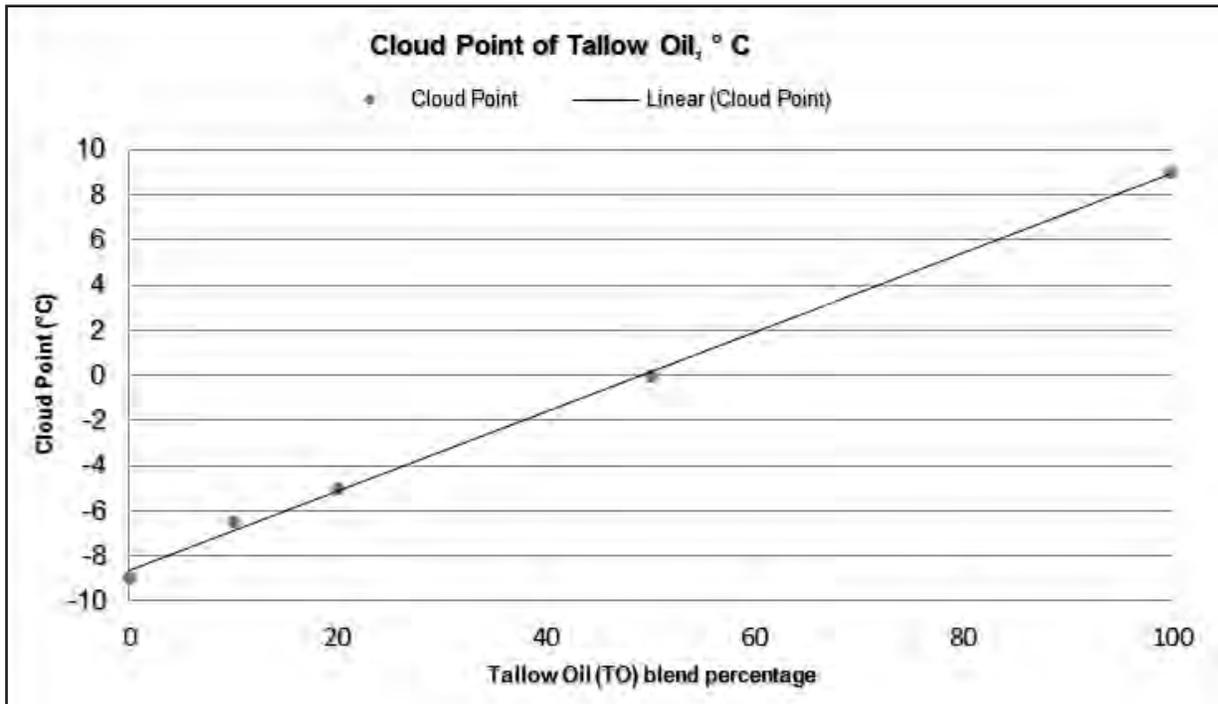


Figure 12. Linearity Figure for Cloud Point of TO

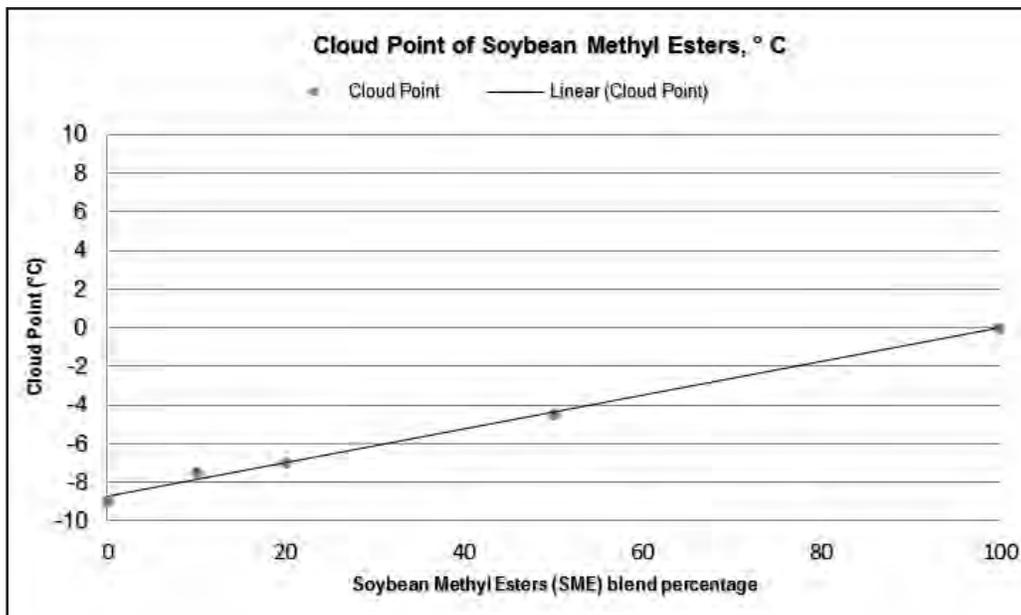


Figure 13. Linearity Figure for Cloud Point of SME

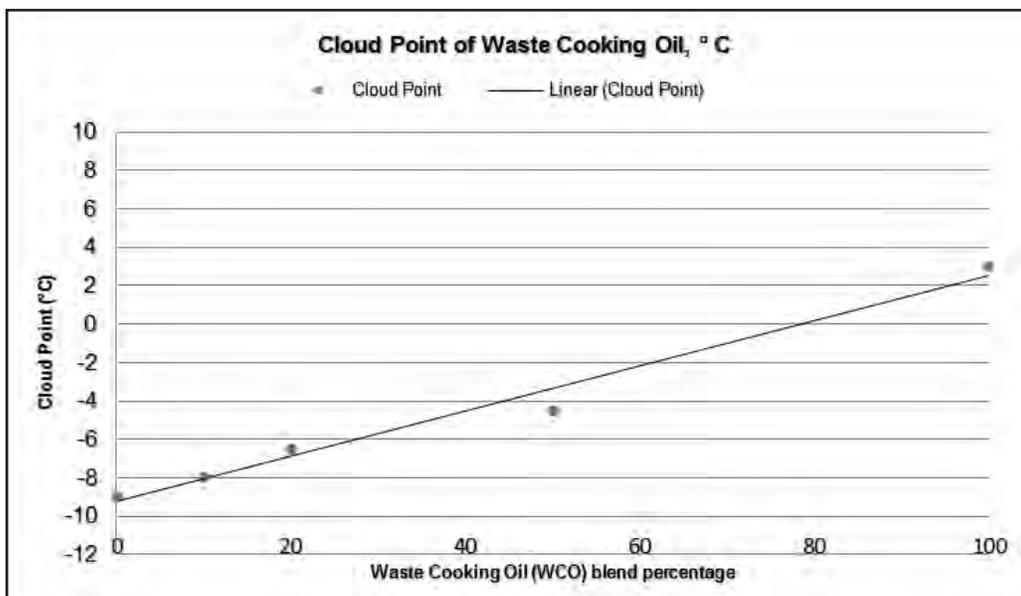
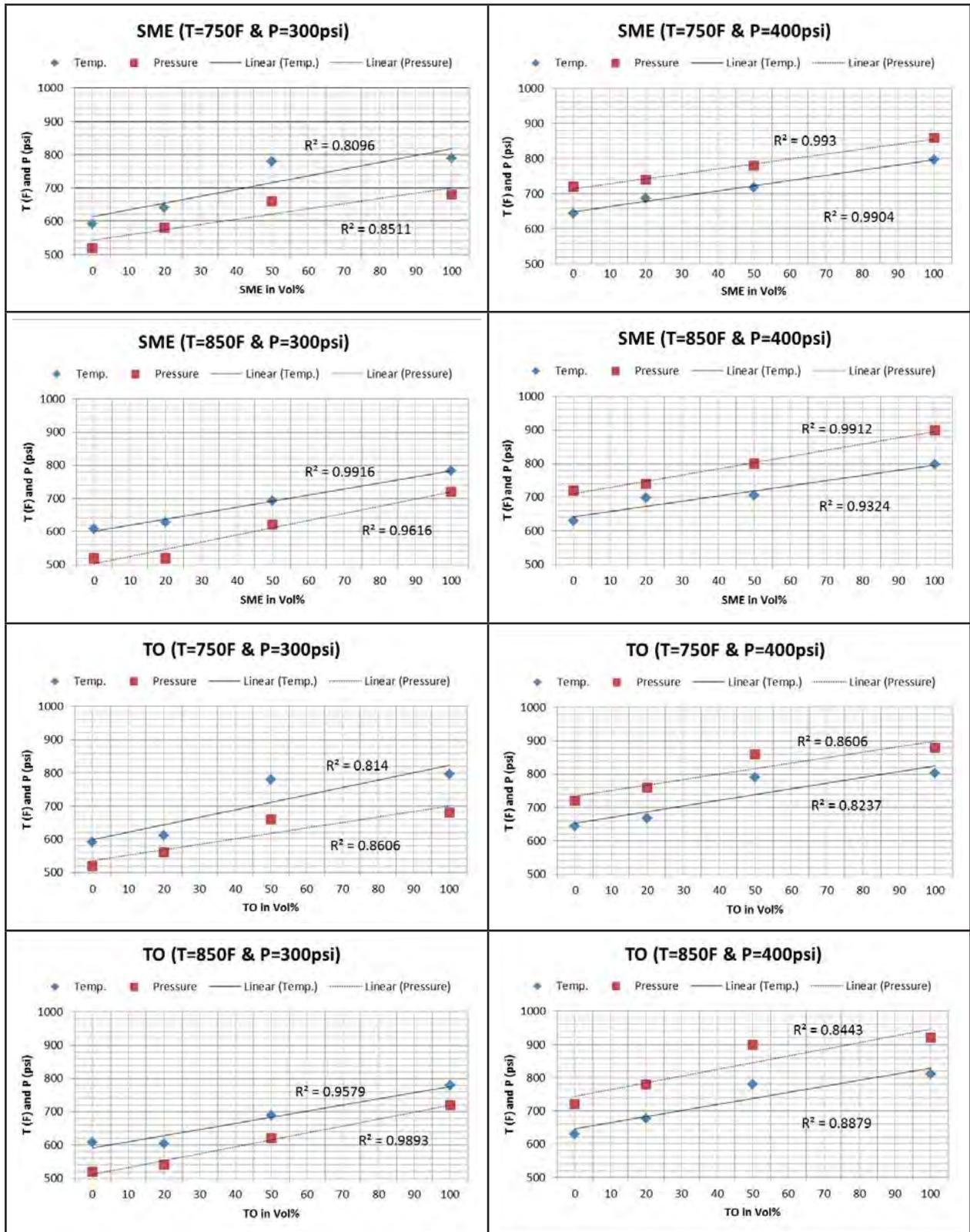


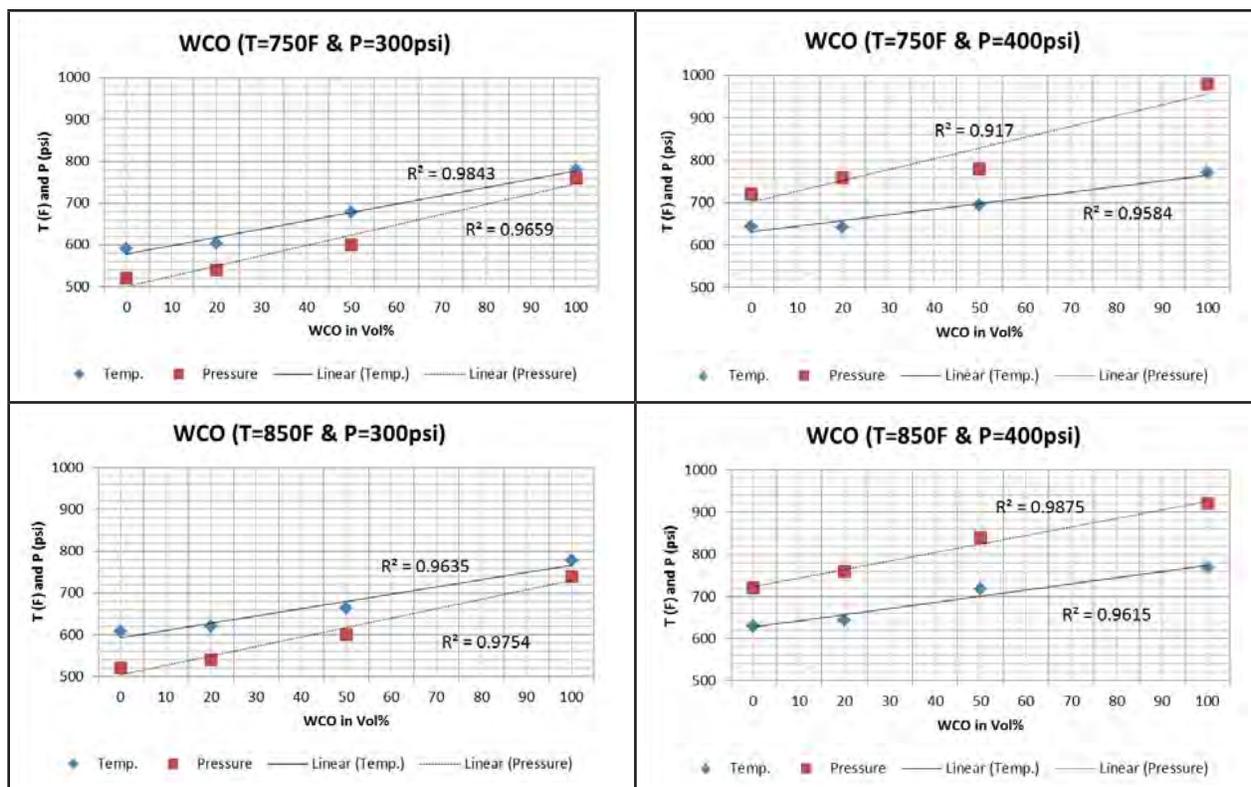
Figure 14. Linearity of the Data for Cloud Point of WCO Biodiesel

## Combustion Process Variables and Correlations

Combustion of different biodiesel samples and ULSD at different temperatures and pressures was carried out, and the results showed linear relationships between the samples and combustion conditions ( $R^2 > 0.8$ ). Both T and P varied linearly as the biodiesel blending percentage in volume was changed. Combustion of pure biodiesel (B100) showed higher T and P after combustion in any set points. The reason may be the high oxygen content of the biodiesel, which raised the combustion points to reach higher T and P as shown in Figure 15. In addition, due to the limitations (maximum operation temperature and

pressure) of the combustion chamber, and safety precautions, combustion temperature and pressure were predetermined as the values shown in Figure 15. All of the graphs are plotted in the same scale so that all three biodiesel fuels and their blends can be easily compared. The Y-axis demonstrates both temperature (in °F) and pressure (in psi).





**Figure 15. Combustion T/P of Different Fuels and Feedstocks at Specified Conditions**

The highest combustion temperatures—around 800 °F—were observed in all pure biodiesel fuels. A lower combustion temperature (600 °F) was observed for ULSD. Again, this is due to a lack of oxygen in ULSD and high oxygen content in biodiesel. The benefit of using biodiesel is an improvement of roughly 7% in combustion efficiency. However, biodiesel has less energy content than regular diesel. In other words, the calorific value of biodiesel is around 37 MJ/kg, which is approximately 9% lower than that of ULSD.

Although the different biodiesel fuels have different compositions, they showed the same trend and relatively the same results at the defined conditions. Consequently, variations in biodiesel energy density depend more on the type of feedstock than on combustion conditions. The effects of temperature, pressure, feedstocks, and blends on emission conditions are presented in following sections.

## Elemental Analysis

Many metals and inorganic elements have been reported to originate from various sources in fuel and engines, making it difficult, if not impossible, to determine the major sources of the elements found in PM in real-world systems. Therefore, it was determined that a detailed analysis of the observed elements would provide a better understanding of possible sources. All of the detected elements in the lab experiment were produced from the combustion of fuel itself; no additional combustible materials, such as engine parts, lubricants, oil, special gaskets, etc. were present. The lab results from a combustion chamber are comparable to the PM elemental analysis of field experiments. The results

were collected at a temperature range of 750 °F to 850 °F and a pressure range of 300 psi to 400 psi. Each section of Table 11 contains the elemental analysis result of biodiesel fuels and blends with ULSD. Comparing results from a range of experiments is more useful than the results at a single point.

Table 11 shows the distribution of PM elements. The concentration of the elements may be considered in relation to the nature of the fuel used. The elemental analysis of the exhaust PM was carried out, and 11 elements were detected in the samples at the different temperatures and pressures. The most abundant elements found in all combustion conditions were alkali metals, specifically, Calcium (Ca) and Sodium (Na). Concentrations of other detectable elements, such as Al, B, Cr, K, Mg, Ni, and Si, comprised approximately one third of the total emission composition.

Al, Cr, Mg, and Si were emitted in the same relative concentrations in all cases. From these results, as well as those of a previous study,<sup>61</sup> it can be concluded that Ca and Na, are the elements emitted in greatest abundance from combustion of these fuels.

**Table 11. Elemental Analysis of Collected PM Samples from Laboratory Reactor [in ppb]**

ppb	ULSD	SME	TO	WCO
Al	0.044±0.013	0.034±0.005	0.046±0.006	0.029±0.009
B	ND	ND	ND	0.041±0.001
Ca	0.160±0.036	0.187±0.069	0.200±0.061	0.285±0.049
Cr	0.024±0.000	0.029±0.004	0.023±0.001	ND
Fe	0.066±0.017	0.121±0.042	0.111±0.050	0.093±0.036
K	0.046±0.000	ND	ND	ND
Mg	0.059±0.000	0.052±0.035	0.064±0.031	0.075±0.017
Na	0.637±0.073	0.643±0.266	0.687±0.103	0.030±0.012
Ni	ND	ND	0.022±0.000	ND
S	0.069±0.008	0.069±0.029	0.083±0.012	ND
Si	0.029±0.002	0.031±0.008	0.038±0.025	0.035±0.002

ND: Not detected.

Each element and its concentration may indicate a specific source. In Table 11, for pure biodiesels, the elements with noticeable concentrations, such as Ca, Fe, Na, and S are thought to come mainly from the tested fuel itself; the contribution from the combustion chamber parts should be negligible, and no fuel additives were used. For ULSD, these metals may come from fuel additives, since fuel additives are used to enhance the physical/chemical properties of diesel.

It can be concluded that, regardless of fuel type, Al, B, Ca, Cr, Fe, K, Mg, Na, Ni, S, and Si were the main detected elements under the given combustion conditions. The characteristics of PM elements from both ULSD and biodiesel are relatively similar when combusted in very low volumes.

Emission of these elements can be reduced in real systems by minimizing PM formation during combustion. Major contributors to PM formation can be identified using PM formation modeling. Filters or post-treatment technologies can reduce elemental emissions to the range of nanograms per cubic meter or even lower.

The morphology of atmospheric particles has received substantial attention in recent years due to the significance of the particles' shape to their impacts on human health.<sup>138</sup> The morphology results showed that the collected PMs were in the form of aggregate rather than single particles. This may be explained by their retention time. In real combustion systems, PM is released in a short period of time, but here, the combustion process took much longer from ignition to sample collection. More collisions were expected, resulting in the formation of larger particles with sizes ranging from 20-100  $\mu\text{m}$ , as shown in Figure 16. Dominant morphological types were categorized as deformed/agglomerated particles (unknown shape), squares, rectangles, and strings. Some micrographs of PM samples obtained by the ESEM are shown in Figure 16.



**Figure 16. ESEM Images of Selected Large PM Samples**

## FIELD EXPERIMENTS

According to USEPA standards presented in Table 4, diesel engines have undergone several phases of development with regard to exhaust emissions. To meet environmental and health regulations, a series of changes in fuel injection systems and compression ratios have been required, in addition to modification of fuel properties. These efforts have led to a lowering of the emission of TPM and number of particles caused by unburned or partially burned fuel.

## TPM Analysis

Ten transit buses powered by Cummins engines were tested in this study and the results are compared with the literature data. No modifications in engine or fueling system were made on the TARTA vehicles to run on biodiesel. Table 12 shows the comparison results of several samples from 700 and the 800 series fueled with B20 in two idle modes. The test results with very narrow error ranges proved the credibility of the PM emissions testing conducted in this study. Biodiesel blend, B20, have a significant effect on PM emissions compared with ULSD. The PM concentrations were evaluated gravimetrically (weighting the filters before and after sampling) and are compared with a previous study.<sup>62</sup> Table 12

shows the PM concentration per unit volume of the exhaust flow rate for different bus series at minimum load (less than 10%). A complete analysis was done first by choosing a large population of different on-road buses running on B20. The results were compared with a previous study<sup>62</sup> in which the authors investigated only two buses that ran on both B20 and ULSD with the limited number of tests. The findings in this study can be a good representation of PM characterization from urban transit buses in idle modes. It is worth mentioning that since last year, all TARTA transit bus fuels were replaced with B20 and none of them have used ULSD since then. Therefore the results obtained in this study only cover B20 emissions.

**Table 12. Comparison for TPM ( $\mu\text{g}/\text{m}^3$ ) for Three Different Transit Series Fueled with ULSD and B20<sup>a</sup>**

	500's series <sup>62,a</sup>				700's series <sup>a</sup>		800's series <sup>a</sup>	
	ULSD		B20		B20		B20	
	Hot	Cold	Hot	Cold	Hot	Cold	Hot	Cold
Mean	215.6±33.4	152.8±41.6	209.8±33.0	127.4±47.9	1.56±0.79	2.37±1.35	0.63±0.12	0.43±0.26
Min.	149.67	106.16	164.49	53.93	0.38	0.42	0.42	0.014
Max.	247.49	218.27	249.57	200.68	2.77	5.59	0.70	0.98
n	7	7	7	7	20	20	6	20

<sup>a</sup> Results presented here are for five buses in both 700 and 800 series. Exhaust flow rate is considered based on Donaldson Engine Exhaust Flow Guide.

As shown in Table 12, the difference between the B20 and ULSD emissions is very clear and the results of the PM analysis show that the 500 bus series emitted PM at substantially higher concentrations than either the 700 or 800 series. It means that the PM mean value was dependent on the engine operating mode and fuel type, but the effect of the catalytic converter should not be ignored. Previous studies showed that use of the biodiesel blends with a catalytic converter had reductions of 50–80% in TPM compared to the emissions with the diesel fuel without a catalytic converter.<sup>139</sup> It is worth mentioning that the standard deviation (SD) values presented in Table 12 come from not only a bus, but also different buses with the same engine type and relatively the same mileage.

The reported PM average mass emissions range from 106.16 to 218.27  $\mu\text{g}/\text{m}^3$  for cold idling and from 149.67 to 247.49  $\mu\text{g}/\text{m}^3$  for hot idling when the 500 bus series were running on ULSD.<sup>62</sup> The orders of magnitude of the average PM mass were the same when fuel was replaced with B20 for Mercedes Benz engines, but a slight decrease was observed in values. The PM values range from 53.93 to 200.68  $\mu\text{g}/\text{m}^3$  for cold idling, and from 164.49 to 249.57  $\mu\text{g}/\text{m}^3$  for hot idling, of which the authors mentioned that those buses did not meet the USEPA emission 2010 standard.

The mass values of collected PM in two new bus series showed a sharp reduction in PM mass compared to the result in the literature. In cold idle mode the PM range was found between 0.42 and 5.59  $\mu\text{g}/\text{m}^3$  for the 700 series and 0.014 to 0.98  $\mu\text{g}/\text{m}^3$  for the 800 series. The trend is the same for hot idling as well, which was 0.38 to 2.77  $\mu\text{g}/\text{m}^3$  for the 700 series and 0.42 to 0.70  $\mu\text{g}/\text{m}^3$  for the 800 series.

The low PM emissions from biodiesel are due to the characteristics of biodiesel, such as higher oxygen content and higher viscosity of biodiesel than ULSD that can break fuel-rich zones in a combustion media.<sup>140,141</sup> Lower sulfur content of biodiesel could be another reason for the reduction. It is worth mentioning that a minimum load was considered as a base scenario for idle tests in this study. On the other hand, at a low load, viscosity would become a primary factor because of the inferior vaporization and atomization at low temperature. Wu et al.<sup>142</sup> explained that at a high load, oxygen in biodiesel is the control factor for locally fuel-rich regions, and oxygen has a more significant impact on combustion.

In addition, as shown in Table 1 and biodiesel property tests, the higher viscosity and density of biodiesel compared to ULSD may lead to an increase in the injection pressure that enhances uniform distribution of fuel in an engine. Likewise, the higher bulk modulus of compressibility of methyl esters in biodiesel can lead to advanced injection timing. As a result, biodiesel fuel enters the combustion chamber relatively quicker than ULSD. This advancement in the combustion process of biodiesel increases the residence time of soot particles in the combustion chamber, thus they undergo further oxidation leading to reduction in PM formation.

To sum up, the reduction in PM emissions when using biodiesel can be attributed to the following:<sup>143</sup>

- Absence of aromatics, which are considered soot precursors in biodiesel
- High oxygen content, which enhances the combustion process
- Lower stoichiometric need for air in combustion reduces the probability of fuel-rich region in a mixture with non-uniform fuel/air ratio
- Nil amount of sulfur compared with regular diesel, which prevents sulfate formation (significant component of typical diesel PM), and scrubbing effect by which sulfur becomes an active center for HC adsorption on the surface of soot

## Elemental Analysis

Elemental analysis was conducted to better understand the health effects associated with PM emissions, and to develop a relationship between the PM chemical structure and the sources of the particles. Different biodiesels were combusted in a laboratory reactor and the collected PM were analyzed for their elements. Laboratory analyses showed that only Al, B, Ca, Cr, Fe, K, Mg, Na, Ni, S, and Si, were completely emitted from 100% biodiesel. Now in a series of real engines, tests were performed on the samples of ten public transit buses, operated for 15 minutes in cold and hot idle modes. To enhance the quality of the results, as mentioned in methodology, blank filters were collected during sampling. The concentrations of Al, Ca, Cr, Cu, Fe, Pb, Mg, Mo, Ni, P, K, Si, Na, S, and Zn were determined in all the above samples using ICP-OES. All the comparisons made for the tested series are shown in Table 13 in detail. The concentrations of the elements which were detected well below the threshold value of the instrument were not considered for the analysis. It should be noted that the concentrations were calculated based on a maximum flow rate.

**Table 13. PM Elemental Composition (ng/m<sup>3</sup>) Collected from Tail Pipe Emission of TARTA Buses**

	500 series (cold Idling)		700 series		800 series	
	ULSD (Avg.)	B20 (Avg.)	Cold Idling B20 (Avg.)	Hot Idling B20 (Avg.)	Cold Idling B20 (Avg.)	Hot Idling B20 (Avg.)
Aluminum (Al)	8.1	16.2	25.75±18.37	11.79±3.34	0.30±0.00	0.01±0.00
Calcium (Ca)	165.4	215.5	335.57±165.70	97.68±35.65	0.35±0.11	0.15±0.06
Chromium (Cr)	0.4	0.7	ND	6.68±0.31	ND	0.01±0.00
Copper (Cu)	0.9	2.6	ND	ND	ND	ND
Iron (Fe)	36.8	48.5	43.29±24.44	35.91±15.51	0.05±0.03	0.04±0.01
Lead (Pb)	0.7	1.3	ND	ND	ND	ND
Magnesium (Mg)	ND	86.1	33.26±12.56	8.73±3.66	0.03±0.02	0.01±0.00
Molybdenum (Mo)	1.3	3.2	ND	ND	ND	ND
Nickel (Ni)	1.3	5.2	ND	ND	ND	ND
Phosphorus (P)	32.6	60.7	22.13±9.25	8.69±2.17	ND	ND
Potassium (K)	ND	ND	ND	ND	0.31±0.00	0.02±0.02
Silicon (Si)	200.5	284.2	ND	37.31±4.74	ND	0.04±0.01
Sodium (Na)	NR	NR	26.13±25.78	183.60±14.14	0.02±0.01	0.18±0.02
Sulfur (S)	NR	NR	27.06±14.01	32.59±3.66	0.03±0.01	0.03±0.00
Zinc (Zn)	29.4	71.1	20.06±5.94	13.21±3.91	ND	0.01±0.00
#			20	20	20	6

Notes:

NR: Not Reported by the author.

ND: Not Detected (When the elements concentration were below the quantitation limit).

More parameters are involved in real engine combustion study, therefore more elements are detected. This is the reason why both laboratory experiments and real engine combustion are conducted.

Sulfur has an important role in the self-lubricating properties of diesel; hence, for ULSD, the wear-generated metal concentrations would be possibly even higher than for regular diesel.<sup>144</sup> It is thought that the low caloric value of biodiesel may have led to higher volumetric fuel consumption for the same load and speed than ULSD.

An experimental study for low load operating conditions showed that there were some metals that came from the fuel, which were found in excess in the exhaust. On the other hand, there were some other metals (Mg, Cr, and K) which were found in small quantities. The results indicate that there were some metals such as Mo, and Ni found in the 700 series and not found in the 800 series, whereas some other metals, Cr, K, and Si, were found in hot idle mode and not found in cold idle mode. Ca, and Fe, and Si were reported as the three most abundant elements in ULSD (an average of 84% of mass) in public transit buses, whereas Ca, Fe, Mg, P, Si, and Zn were observed as the most abundant elements for B20 (an average of 96% of mass) in the 500 bus series in cold idle mode.<sup>62</sup> Sometimes lubricants may get into engines and they become as a secondary source for some elements in the exhaust.

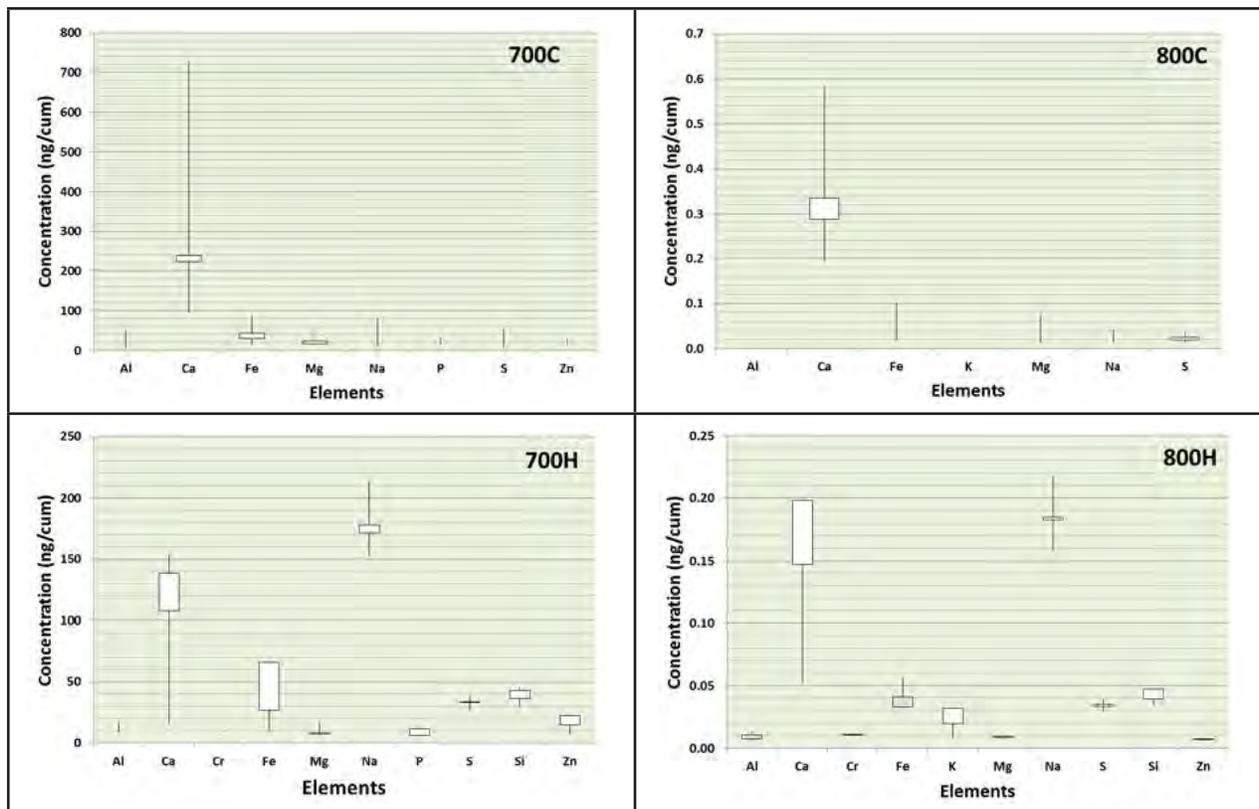
It was observed that Ca was the most abundant element in cold idle mode; for the 700 series the average mass of Ca was 76%, and it was 82% for the 800 series. On the other hand, for the hot idle test, dominant elements were observed Na and Ca with 71% in mass for the 700 series and 72% for the 800 series. Ca is reported as a typical marker for exhaust emission in varying engine types.<sup>145,146</sup> The higher values of Ca may be contributed by the various sources like wear in bushings, injector shields, coolant core tubes, thrust washers, valve guides, connecting rods, piston rings, bearings, sleeves, bearing cages, detergent additives or dust.<sup>62,145,147</sup> Ca is also found in abundance in diesel (902.3 µg/g), biodiesel (721.2 µg/g) and lubricating oil (2046.8 µg/g).<sup>145</sup>

In laboratory experiments, Na was found as one of the dominant elements emitted from the fuels. On the other hand, the possible sources of sodium (Na) in transit buses could be specific additives in lubricant oils.<sup>74</sup> The values of Na for hot idling are higher than for that of cold idling, and its concentration is the highest compared to all the other metals in hot idling. A higher engine temperature is thought to be the main reason for releasing more Na in hot idle mode.

Fe, Mg and S are detected in high concentrations (15-19% mass-based) in cold idle mode. Also Fe, S, and Si were observed for hot mode with 23-24% mass-based. Sharma et al.<sup>74</sup> reported that the concentrations of crustal elements Fe (258 µg/m<sup>3</sup>), Mg (125 µg/m<sup>3</sup>), Ca (936 µg/m<sup>3</sup>) were much higher than those of Cr, Ni, Pb, Zn, Ba and Cd (anthropogenic elements). Regardless of fuel sources for Fe, Mg, S, and Si, possible sources for these elements are:<sup>145,147,148</sup>

- Iron (Fe) came from the wears in the engine block, cylinder, gears, cylinder liners, valve guides, wrist pins, rings, camshaft, oil pump, crankshaft, ball and roller bearings, rust or might be contributed by dust. Note that the diesel has 402.3 µg/g, biodiesel has 419.8 µg/g and lubricating oil has 827 µg/g irons in the fuel.<sup>146</sup>
- Magnesium (Mg) came from cylinder liner, gear box housings and detergent inhibitors.
- Sulfur (S) came from the wears in the engine block, cylinder, gears, cylinder liners, valve guides, rings, camshaft, oil pump, crankshaft, ball and roller bearings, rust for ferrous and the small amount of sulfur (<15 ppm) in ULSD.
- Silicon (Si) came from dirt intrusion in improper air cleaner and seal materials which were found in high concentration in 500 series in cold idle and not found in the 700 and 800 series in the same mode. The Si concentrations in PM collected from the exhaust of the ULSD fueled bus were higher than the concentrations in PM collected from the exhaust of the BD fueled bus.

Figure 17 represents the box plots of elemental analysis for two recent transit buses run on B20 in cold and hot idle modes. The differences in Ca between hot and cold idle modes were also an order of magnitude higher in both the 700 and the 800 series. Therefore, the 800 series in cold mode produced the highest Ca concentration.



**Figure 17. Elemental Analysis for the 700 and 800 Bus Series in both Cold and Hot Idle Modes**

Mo and Ni were detected in small amounts, but Pb and Cu that were found in the 500 series were not detected either here or laboratory experiments. The higher values of Cr and Si in hot idle may be affected by higher temperature during hot idle mode. The 500 series (both running on ULSD and B20) exhaust particulates showed relatively high levels of P concentration, where the 700 series showed trace concentrations of P in the particulates. However, the 800 series displayed no P concentration in elemental analysis.

Results of testing for other metals such as Ag, Ba, Cd, Co, Cu, Mn, Mo, Pb, Sb, Sr, Ti, and V, which were published before<sup>142,149</sup> were not detected in this study. This means that those elements did not have the same sources in the present study. A study by Wang and Huang<sup>150</sup> showed the same results. They reported that Al, Ca, Fe, Mg, and Si (crust elements) were much higher than anthropogenic elements (such as Pb and Cu). By implementing a correlating matrix to find the elements with the same possible sources, Shandilya and Kumar<sup>71</sup> concluded that due to a positive correlation between some elements (for example Zn and P), both are regarded to come from a single source.

To better analyze the results, PMF was used to elucidate sources of PM collected in TARTA garage, Toledo, OH. PMF, a multivariate factor analysis tool, decomposes a matrix of speciated sample data into two matrices (factor contributions and factor profiles). One of the unique advantages to PMF is the ability to handle data that is missing or below detection limits. More information regarding PMF is presented in the report by Noris et al.<sup>122</sup> The main parameters in PMF are the number of factors that define the species profile and

mass contribution to each factor properly.<sup>120</sup> Most repeatable elements were considered for the PMF analysis, and other elements which are not presented in Table 14 were not selected because of their low and very low signal-to-noise ratios (S/N), and concentrations.

The number of factors (p) was selected based on an analysis of model fitting, Q, numbers of samples, procedure and the data. The numbers of runs and seed count were kept the same as default values. Fuel, oil and lubricant, engine parts, and ambient source were taken as four main sources in elemental characterization. Table 14 summarizes the contribution of different source profiles after the analysis.

**Table 14. Percent Contribution of Four Common Sources in PM Elemental Analysis**

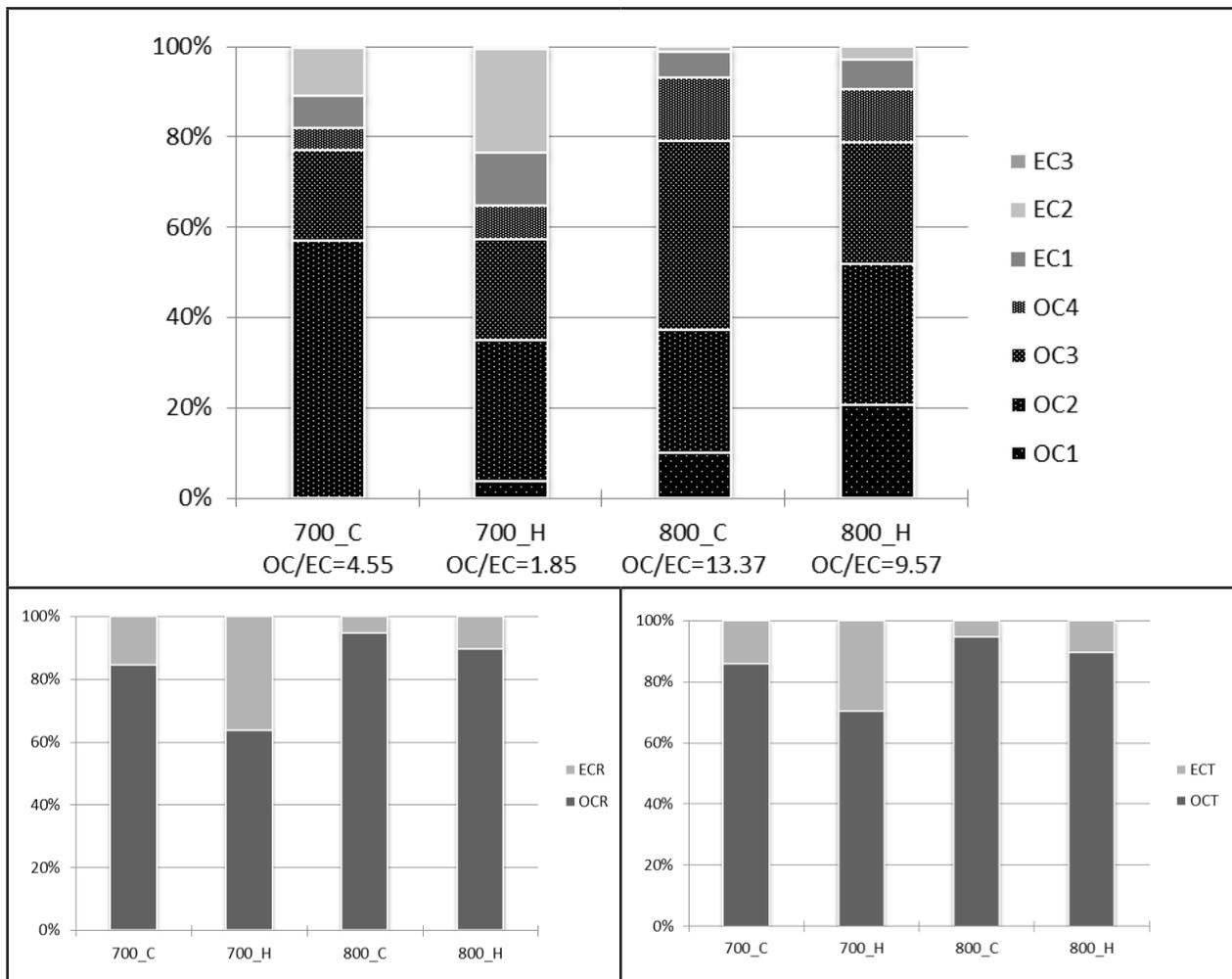
	Elements	Fuel	Oil and lubricant	Engine parts	Ambient
700C	Calcium (Ca)	18.5	7.3	9.0	65.2
	Iron (Fe)	14.2	2.0	83.2	0.7
	Magnesium (Mg)	0.0	84.8	0.0	15.2
	Sulfur (S)	85.7	1.5	0.0	12.8
700H	Calcium (Ca)	22.5	43.5	9.4	24.5
	Iron (Fe)	0.0	44.6	55.4	0.0
	Sodium (Na)	44.1	0.4	38.1	17.4
	Phosphorus (P)	5.7	94.3	0.0	0.0
	Sulfur (S)	35.3	11.5	33.3	20.0
	Silicon (Si)	25.3	0.0	38.2	36.5
800C	Zinc (Zn)	0.0	70.8	0.0	29.2
	Calcium (Ca)	11.3	17.8	7.6	63.3
	Magnesium (Mg)	8.9	84.9	6.2	0.0
800H	Sulfur (S)	50.5	0.0	26.0	23.5
	Aluminum (Al)	0.0	27.1	2.1	70.7
	Calcium (Ca)	26.3	57.7	8.3	7.7
	Iron (Fe)	0.0	3.6	96.4	0.0
	Sodium (Na)	34.8	9.3	15.4	40.4
	Sulfur (S)	34.7	21.1	13.1	31.1
	Silicon (Si)	11.6	24.9	38.9	24.6

A detailed description of types and sources is presented above and in Table 14. PMF study showed that the fuel source significantly contributed to the emissions of Sulfur (S), Calcium (Ca) and somewhat Sodium (Na), respectively. Magnesium (Mg), Phosphorus (P), Zinc (Zn) and somewhat Calcium (Ca) had significant portion in oil and lubricant as shown in Table 14. These elements are usually used to enhance the quality of oil and lubricant as described earlier. Aluminum (Al) which was detected in a few cases is considered as an indicator of dust when gets into a storage tank.<sup>62</sup>

## Elemental and Organic Carbon

Diesel engine emissions are composed of highly complex mixtures. Wide ranges of organic and inorganic compounds were found in the gaseous and particulate phases. Diesel exhaust particulates are mainly composed of carbon that occupies a dominant portion (about 80-90%) of DPM concentration and mainly exists in the form of EC and OC.<sup>151,152</sup> EC (called Black Carbon or “BC,” a nonvolatile and strongly light-absorbing portion) is a carbonaceous core of DPM that is emitted during the combustion of fuels as small, soot-like particles, often with other chemicals attached to the surface. Sources of OC (volatile and light-scattering portion) include traffic, industrial combustion and the degradation of carbon-containing materials. Both contribute to the toxicity of DPM, and also to regional visibility impairment and climate change.<sup>153,154</sup>

The EC and OC emissions in the collected PM for two different bus series and two idle modes with low engine loads are shown in Figure 18. The figure presents average concentrations. Detailed values of carbon emissions are also presented in Table 15. The results of this study and previous study on both ULSD and biodiesel show that EC is emitted in a much lower value than OC. Biodiesel and ULSD emissions analyses indicate that these fuels could effectively reduce the emission of EC. The trends are completely in agreement with earlier studies.<sup>71,73</sup>



**Figure 18. Fraction of Different Carbon Components in the Total Carbon in both Hot and Cold Idle Modes with OC and EC (Reflectance and Transmittance) Percentage in Total Carbon**

It can be seen that EC was reduced to less than 10% by switching from the 700 to 800 series at idling conditions, while OC gradually increased to 90% at minimum load (<10%). The values of EC1, EC2, and EC3 for the 800 series in both cold and hot idle modes showed the same values and ratios as shown in Figure 18. For the 700 series, by increasing the engine temperature to hot idle mode, more EC was released compared with the cold idle mode. The maximum amount of observed EC in this case was reported as 35% of total carbon (TC=EC+OC).

The results suggested that temperature can increase the share of EC in the 700 series, but after treatment methods in the 800 series lead to the relatively same OC/EC ratios in both hot and cold idle modes.

EC is known to be formed in the fuel-rich zone under high pressure and temperature. Cheung et al.<sup>73</sup> suggested that the oxygen content of biodiesel inhibits in-cylinder soot production by disrupting the carbon chain development and promoting oxidation. Additionally, Wu et al.<sup>142</sup> suggested that more OC emission be found at the low engine load due to lower fuel-

to-air ratio. In this case, physical properties like volatility might become the dominant factor rather than the fuel oxygen content in particle formation. The result of this study is in total agreement with above statements and shows that hot idle mode can enhance the amount of EC emissions compared to OC.

**Table 15. Carbon Emissions from Transit Buses in Three Different Bus Series**

( $\mu\text{gC}/\text{m}^3$ )	DPM AVG	OC	EC	TC	CF	OC 1	OC 2	OC 3	OC 4	EC 1	EC 2	EC 3
700_C_BD	7.57	5.91	1.29	7.20	1.11	0.05	4.05	1.46	0.35	0.51	0.76	0.02
700_H_BD	2.90	1.49	0.80	2.29	0.89	0.09	0.72	0.51	0.17	0.26	0.53	0.01
800_C_BD	0.81	4.25	0.32	4.57	6.69	0.46	1.24	1.92	0.63	0.27	0.05	0.00
800_H_BD	2.79	3.61	0.38	3.99	1.69	0.83	1.24	1.07	0.47	0.27	0.11	0.00
500_H_ULSD	149.67	99.89	13.71	113.60	0.89							
500_C_ULSD	142.94	87.73	22.46	110.19	0.87							
500_H_BD	206.83	145.25	10.68	155.93	0.90							
500_C_BD	117.91	73.81	13.46	87.27	0.84							

Note: Average values are reported here. Data for 500 bus series were reported from a previous study.<sup>72</sup>

Carbon is stored in the form of EC1, OC1 and OC2. EC1 (called char-EC) was formed directly from pyrolysis of fuel at a relatively low temperature, and EC2+EC3 (or soot-EC) could be used as the trace composition for diesel emissions.<sup>155,156</sup> Soot-EC was formed via gas-to-particle conversion at high combustion temperature.<sup>72,155</sup> The OC1-OC4, and EC1-EC3 emissions, as well as OC, EC, and TC, are presented in Table 15. As shown in this table, carbonaceous emissions from both 700 and 800 series were significantly lower than in previous studies.<sup>71</sup> Shandilya and Kumar<sup>71</sup> reported that for ULSD fueled buses, EC2 was the major exhaust of regular diesel vehicles (32.5% of TC), and OC2 was the major exhaust emission for biodiesel-fueled buses (42.7% of TC). In the present study, the results totally satisfied the above statement, especially for the 700 series in both hot (31.4% of TC) and cold (56.25% of TC) idling. Furthermore, it can be inferred that biodiesel as a fuel is very successful in eliminating the toxic component of EC from diesel, primarily due to presence of oxygen in fuel. The CF value was reduced to approximately between 0.89 to 1.69 except for 800's cold idling.

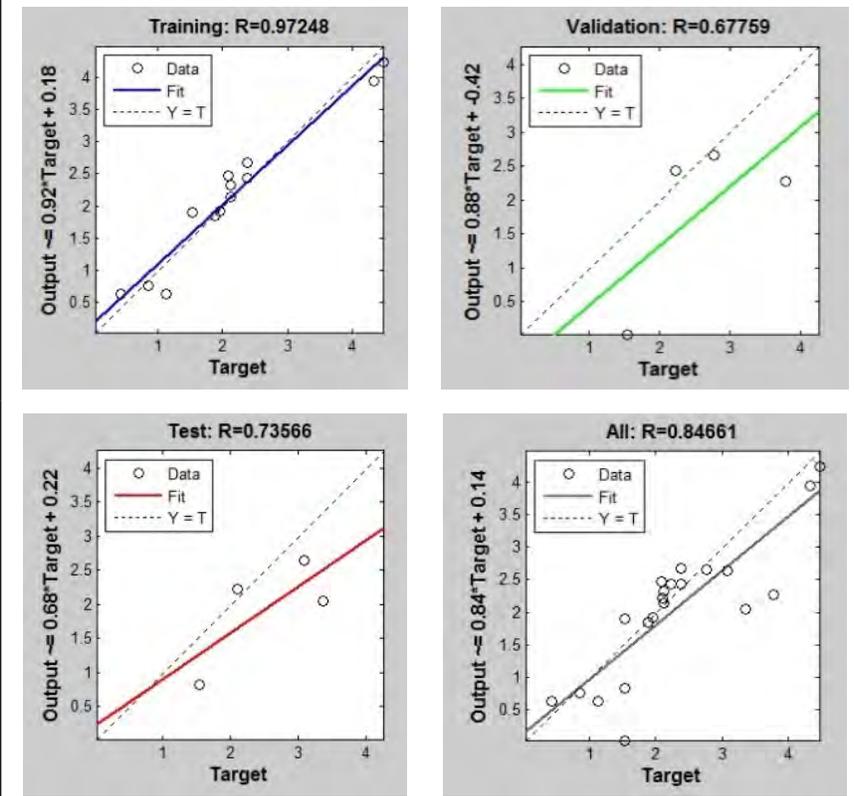
## MODELING

### Neural Network

Neural network maps between inputs and outputs were used here, along with a two-layer feed-forward network with sigmoid hidden neurons and linear output neurons. The collected PM from transit buses on quartz filter papers was converted into mass concentration. Sampling was done from mid-July 2012 through November 2012 in Toledo, OH. All the input parameters were used in the ANN simulation to accurately predict the PM in the exhaust. A portion of input data (30%) was set aside for validation/testing the network.

These data are fitted using the ANN strategy stated above under the explained conditions. The predicted and experimental values of particle concentration are shown in Figure 19 for both 700 and 800 bus series. All the input parameters, which were gathered during the sampling from engines, were used to predict PM concentrations. As can be seen in these figures, the comparison of the predicted values and experimental measurements shows agreement between the predicted and experimental data. The correlation coefficients,  $R^2$ , of the PM concentrations were 0.97 and 0.92 for 700's and 800's series, respectively, for the training sets. For the validation and testing sets, the correlation coefficients were 0.68 and 0.74 for the 700 series and 0.99 and 0.76 for the 800 series, respectively.

Experimental and ANN predicted values of particle concentration for 700 bus series, training set, testing set, validation set and all



Experimental and ANN predicted values of particle concentration for 800 bus series, training set, testing set, validation set and all

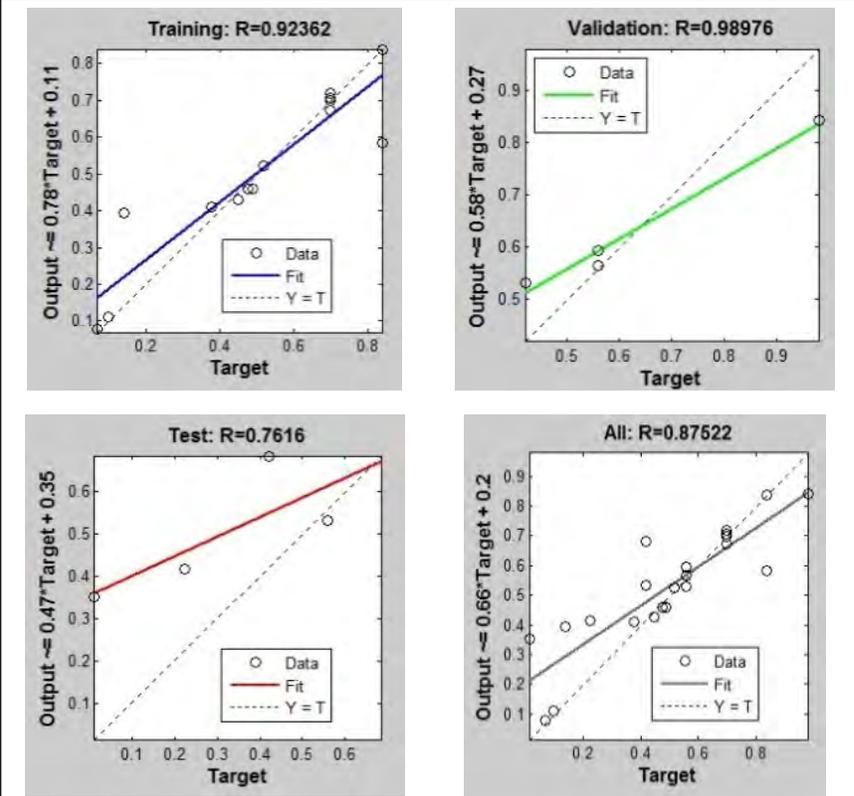


Figure 19. Experimental and Predicted Values of PM Concentrations

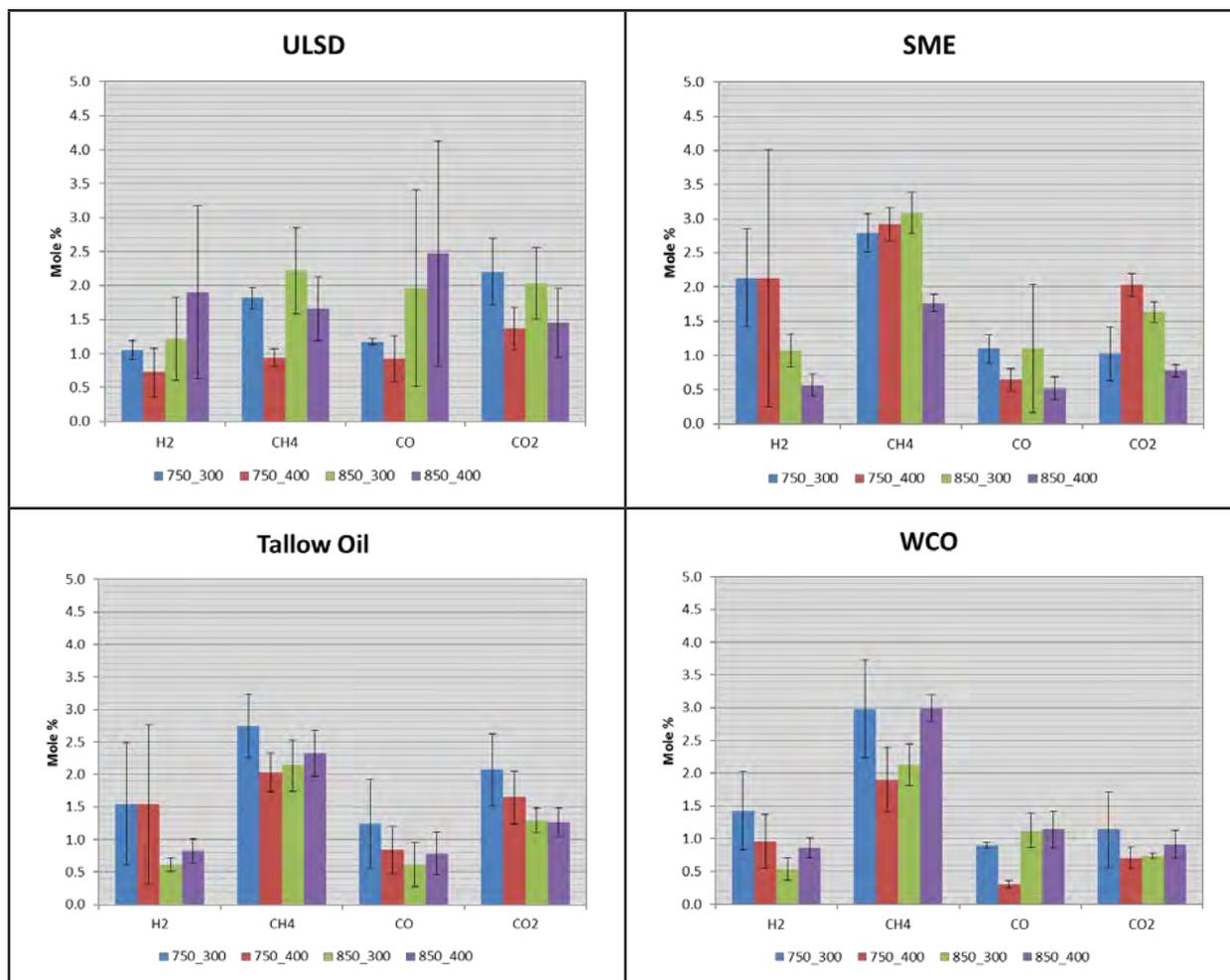
To summarize, it was demonstrated that the idle emissions data could be modeled using ANN methodology, which has the ability to admit approximate reasoning, imprecision, and uncertainty of data. The quality of the model may be improved when a high number of samples are introduced to the system (especially for predicting elemental analyses). The results show that for a complex system which has many input parameters, ANN will be a very practical and feasible model for input-output correlation and ANN is one of the best tools to predict the exhaust emissions.

### Combustion Emission and Modeling

The correct description of chemical changes requires the application of reaction mechanisms consisting of complex sets of reactions. This means that the chemistry of combustion processes is to be described by a huge number of parameters such as temperature, concentration and reaction kinetic data. Comparison of all detected emission gases using GC is presented in Figure 20. The comparison is done for components' concentrations at the combination of predetermined temperature (750 °F and 850 °F) and pressure (300 psi and 400 psi). GC could not detect other HC molecules and only H<sub>2</sub>, CH<sub>4</sub>, CO, CO<sub>2</sub> were detected. Figure 20 shows the emission characteristics of combustion gases from ULSD and three different biodiesel feedstocks. Higher oxygen content of biodiesel makes it possible to promote the combustion process and to increase the combustion temperature. As shown in Figure 20, SME, TO, and WCO produced approximately the same concentrations of CO as ULSD especially at lower T/P, but produced lower CO<sub>2</sub> concentrations than ULSD. The lower emissions of CO and CO<sub>2</sub> are related to lower ratio of carbon to oxygen in biodiesel fuels compared to ULSD.

As far as pollution potential is concerned, the biodiesel blends and pure biodiesel fuels can be considered a more favorable fuel than regular diesel for engine combustion. As seen in Figure 20, the use of oxygenated fuels in the reactor resulted in relatively lower emissions of CO and CO<sub>2</sub>, compared to the emissions from ULSD combustion.

CO emissions are the result of incomplete or partial combustion, and the oxygenated biodiesel fuels emitted the lowest CO concentrations (maximum was 1.3%), which may be attributed to the lower carbon content (by weight) of this renewable alternative fuel compared to other fuels. Figure 20 also depicts the formation of CO<sub>2</sub>, a greenhouse gas, in relation to feedstocks. WCO shows lower emissions of CO<sub>2</sub> for biodiesel fuels. Reduction in CO<sub>2</sub> emissions by using biodiesel fuels can be expected to reduce the hazardous impact on global warming and climate change.



**Figure 20. Effect of Temperature and Pressure on Fuel Combustion**

Fatty acids in SME are mainly composed of linoleic acid which has a different composition from TO, which is mainly composed of oleic acid as shown in Table 3. According to the amount of emission, all three biodiesel fuels emitted relatively the same mole concentrations when the temperature and pressure changed, but SME produced more intermediate products (CH<sub>4</sub>) than the other fuels. Formation of CH<sub>4</sub> as an intermediate combustion species for biodiesel fuels is higher than ULSD. SME showed the highest formation of CH<sub>4</sub> among other biodiesel fuels. High concentration of methane was obtained at higher temperature and lower pressure (3.1%).

The results of the simple MB model are presented in Table 16 for the species of interest. The MB model could not predict the formation of hydrogen very well. The reason for this phenomenon most likely was participation of molecules that were not considered in the reaction schemes. This means more terminating reactions are needed to better simulate hydrogen formation. Simple pathways presented an equal chance of formation for both CO and CO<sub>2</sub> as shown in the Table 16. Overall, descent estimations were obtained from an orders of magnitude point of view. The simulation results summarized in Table 16 show that during the time for complete consumption of oxygen, the predicted values of CO<sub>2</sub> are

in the same order of magnitude as the measured ones. The SME results are shown first in the Table for each element followed by TO and WCO, respectively.

**Table 16. Comparison of Simple Model Results for MB Combustion in Different Temperature Ranges ( $H_2$ , CO, and  $CO_2$ ) with SME, TO and WCO Results (mole %)**

	Lower Temperature		Higher Temperature	
	Experimental (300psi-400psi)	Model	Experimental (300psi-400psi)	Model
$H_2$	1.31±0.84-0.91±0.27	Trace	1.07±0.24-0.57±0.17	Trace
	1.55±0.94-1.54±1.23		0.61±0.10-0.82±0.18	
	1.43±0.60-0.96±0.41		0.53±0.17-0.86±0.15	
CO	1.09±0.22-0.65±0.16	1.58	1.11±0.94-0.52±0.17	1.69
	1.25±0.68-0.84±0.37		0.62±0.33-0.79±0.32	
	0.89±0.04-0.30±0.06		1.12±0.26-1.14±0.28	
$CO_2$	1.02±0.39-2.03±0.17	1.58	1.63±0.14-0.77±0.09	1.69
	2.07±0.55-1.64±0.41		1.29±0.19-1.27±0.22	
	1.14±0.58-0.71±0.17		0.74±0.04-0.91±0.21	

Note:

Trace: The value which is in the range of ppb or lower (for  $CH_4$ ).



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## V. CONCLUSION AND FUTURE WORKS

Based on the results and discussion stated above, the conclusion and future works are presented in three sections: laboratory experiments, field experiments, and modeling.

### LABORATORY EXPERIMENTS

#### Biodiesel Physical Properties

Biodiesel is being industrialized as one of the potential sources of sustainable energy for transportation in the future. Currently its usage lags behind petroleum and diesel fuels. It is not being used as B100—i.e., pure biodiesel—due to a few properties that make biodiesel unfavorable in all weathers and under different engine conditions. Cloud point, kinematic viscosity and flash point are some of those properties whose values depend on the existence of saturated fatty acids, long carbon chains, and the presence of triglycerides. Higher amount of C16:0 and C18:0 series carbons would increase the cold flow properties and reduce the kinematic viscosity. Presence of lightweight carbon chain compounds in the fuel would reduce deposition of compounds and maintain minimum required flash point. Extensive research on the fatty acid alkyl ester compounds is needed to improve the properties of biodiesel. It is SME which is being put to use in many parts of the world as biodiesel fuel in vehicles, since it has better properties than diesel and biodiesels of different feedstocks. Biodiesel properties test results also concludes that SME has better properties than other two types of biodiesels.

#### Combustion Analysis

The laboratory study of combustion of biodiesel blends (B00, B20, B50 and B100) was performed in a batch reactor at the temperature of 750 °F and 850 °F and pressure of 300 psi and 400 psi. Helium was used to elevate the pressure to the desired set points. Conclusions and suggestions of the work done are summarized below.

The combustion temperature and pressure of different blends followed the linear relationship. As the vol% of biodiesel increased from 0 (ULSD) to 100 (pure biodiesel), the combustion temperature and pressure increased linearly proportional to the biodiesel vol%. High oxygen content of biodiesel appeared to improve combustion efficiency and lead to high reaction temperature and pressure.

Al, B, Ca, Cr, Fe, K, Mg, Na, Ni, S, and Si were detected in the combustion analysis under four specific temperatures and pressures. Sodium and calcium were emitted at much higher concentrations than the other elements in all the combinations of combustion conditions. From comparison of laboratory and field experiments, it can be concluded that other elements which were detected in the field experiments and were not detected in laboratory experiments may have external sources such as engine parts, lubricants, oil, and fuel additives.

Experimental results showed high/low temperature and pressure had minimal effects on emissions of S and Si in many cases, and the obtained results were in agreement with

earlier studies. Next to Na, Ca and Fe showed the highest consistent concentrations in all the experiments. The results were in agreement with field experiments for both hot and cold idling.

The experimental study of the combustion of three biodiesel fuels along with ULSD (only pure ones) are performed in a laboratory batch reactor over the series of temperatures and pressures. Biodiesel and its blends showed relatively lower emission of CO and CO<sub>2</sub> than ULSD. Many reaction pathways resulted in lighter HCs formation such as methane. SME presented higher formation of intermediate species than other fuels, and TO and WCO also showed higher concentrations than ULSD.

## **FIELD EXPERIMENTS**

PM emissions from transit buses running on ULSD and biodiesel derived from SME (B20), were investigated in this study. The results of the PM emission analysis show that PM emissions were dependent on the engine modes and type of fuel. The emission characteristics of biodiesel were measured in terms of TPM and elemental analyses of EC, and OC. The results showed that the TPM was related to idle conditions: the number of heavy metals emitted from hot idle conditions was greater than those from cold idling. This means the concentrations of detected elements in low temperatures, i.e., when the engine and fuel were cold, were lower than during hot idling when the engine was warm.

Elemental analysis and PMF were applied to the experimental data to find the source of PM formation. After the fuel, lubricant oil, additives and engine parts were reported as major sources of elemental concentrations in the PM. Four factors were obtained and identified as the possible sources: fuel, oil and lubricants, engine parts, and ambient air. The most repeatable elements in all cases were Ca, Fe, and S, which were consistent with lab experiments.

The oxygenated structure of biodiesel was thought to be the driving force for putting carbon atoms into the combustion pathways, which reduces soot formation both in size and concentration. The oxygen content may appear on soot surfaces and leads to surface burning which causes diameter reduction of soot. The reduced soot formation may lessen radiation from the soot particles which result in elevated reaction temperature (depicted in Figure 15) and more reaction of molecules which contain the above mentioned inorganic and metal elements. Higher temperature reduces fuel kinematic viscosity and the whole process may result in more detectable elements in exhaust.

At the conclusion of biodiesel combustion in transit buses, the results were in agreement with above mentioned findings and literature data. Results indicated that the use of biodiesel could effectively reduce EC and increase the portion of OC emission. OC<sub>2</sub> and EC<sub>2</sub> contained the most portions of OC and EC, respectively, in the biodiesel bus emissions. The main reason for the above statements could be explained by the oxygenated structure of the fuel, engine technology, and the presence of a catalytic converter in the system.

The results indicated that physical properties of biodiesel blends are very important during engine combustion. Higher viscosity causes reduced fuel leakage during injection, which

drives an advance in injection timing and an increase of mass injection rate. Density of the fuels affects the start of injection, injection pressure, fuel spray characteristics, etc. When the fuel temperature changes and enters in an engine with different temperature (hot or cold), fuel acts differently (Figure 15) and the emissions are different.

## **MODELING**

The ANN method can be more practical than simple kinetic models when a conceptual understanding on an overall correlation between the various input data and the output results are necessary. The ANN method along with the kinetic models are expected to help us better understand the PM formation mechanisms and come up with more efficient feedstock preparation and effective operating conditions to reduce PM. Applying ANN to the system showed the acceptable correlation between engine data (as input) and the PM concentration (as output). Engine data were used to prepare the model as well as certified algorithms from literature studies as discussed earlier. The obtained data presented good correlations between experimental and predicted results.



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Parsons Brinckerhoff

**Rose Guilbault (TE 2014)**  
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Association of American Railroads

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Metropolitan Transportation Commission

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**Will Kempton (TE 2016)**  
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Transportation California

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International Union of Railways (UIC)

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American Public Transportation Association (APTA)

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CEO  
California High-Speed Rail Authority

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Dean, College of Business  
San José State University

**Beverly Swaim-Staley (TE 2016)**  
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Union Station Redevelopment Corporation

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National Transit Services Leader  
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**Edward Wytkind (Ex-Officio)**  
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Transportation Trades Dept., AFL-CIO

(TE) = Term Expiration or Ex-Officio  
\* = Past Chair, Board of Trustee

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