



# Experimental Modeling of NO<sub>x</sub> and PM Generation from Combustion of Various Biodiesel Blends for Urban Transport Buses

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**Study results provide additional justification for the use of biodiesel as an alternative fuel.**

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Although it is generally accepted that biodiesel fuel contributes to the reduction of pollutants, biodiesel still needs more study

for better control of combustion emissions and engine performance. Biodiesel has very diverse sources of feedstock, and due to various blends and chemical components, the amount and composition of its emissions vary significantly depending on combustion conditions.

## Study Methods

This research focuses on generation mechanisms of NO<sub>x</sub>, particulate matter (PM), and carbon emissions from low-temperature combustion (LTC) of different biodiesel feedstocks. Experiments compared the emissions of biodiesel of different grades (B0, B20, B50, and B100 biodiesel) with ultra-low sulfur diesel (ULSD) for three types of biodiesel feedstocks: soybean methyl ester (SME), tallow oil (TO), and waste cooking oil (WCO). Laboratory studies were performed by burning biodiesel and then analyzing the exhaust emissions. The exhaust gas was analyzed for NO<sub>x</sub>, and the collected PM was used for further analyses. For chemical characterization of PM, the collected samples from the reactor were analyzed for their possible elements using inductively coupled plasma mass spectrometry (ICP-MS). For further characterization of PM formed in the laboratory reactor, scanning electron microscope (SEM), transmission electron microscope (TEM), Fourier transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA) were used. Laboratory data was supported by field data collected from Toledo area regional transit authority (TARTA) buses both in idling and running modes. The exhaust gas was analyzed using a NO<sub>x</sub> analyzer and a gas chromatograph (GC) to correlate the fuel's properties with emissions. Finally, in a modeling study, artificial neural network (ANN) and stochastic simulation algorithm (SSA) were applied to field and laboratory data, respectively.

## Findings

The results showed that the biodiesel containing more unsaturated fatty acids emitted higher levels of NO<sub>x</sub> than the biodiesel with more saturated fatty acids. A paired t-test showed that neat TO, WCO, and WCO-B50 significantly reduced the formation of NO<sub>x</sub> compared with ULSD and SME-B20. Thus, less of unsaturated fatty acid methyl esters (FAMES) such as TO and WCO is preferable when reduction of NO<sub>x</sub> emissions is desired.

ULSD showed the highest emission of CO and the lowest emissions of CO<sub>2</sub> and CH<sub>4</sub> among the fuels studied. Compared to ULSD, it was found that the use of pure biodiesel fuels reduced CO by a factor of 0.33 and enhanced CO<sub>2</sub> emissions by a factor of three. Biodiesel fuel with a

high degree of unsaturation and high portion of long methyl esters appeared to produce more CO and less CO<sub>2</sub> emissions than those with low degrees of unsaturation and short chain length (such as WCO and TO). The length of FAMEs affects the carbon emissions because shorter chains have a high oxygen-to-carbon ratio.

In a field study, a novel method was introduced to analyze size distribution of PMs emitted from heavy-duty engines. NO<sub>x</sub> emissions were analyzed in both off-road (idle) and on-road tests. The performance of a bus that ran on blended biodiesel (B5) was found to be similar to that of one that ran on ULSD, and drivability was not an issue with blended biodiesel.

Aside from the ANN study, which was conducted on the field data, SSA was applied to the field data to develop a prediction model for NO<sub>x</sub> emissions. In the SSA, a simple biodiesel surrogate was selected, and main combustion pathways for NO<sub>x</sub> were derived by simplifying a skeletal mechanism proposed in the previous study that includes saturated methyl decanoate (MD), unsaturated methyl 5-decanoate (MD5D), and n-decane (ND). The predicted model results were in good agreement with experimental data at LTC conditions for three different biodiesel fuels consisting of various ratios of unsaturated to saturated methyl esters.

### Policy Recommendations

Biodiesel is being industrialized as one of the potential sources of sustainable energy for transportation in the future. The results presented here provide additional justification for the use of biodiesel as an alternative fuel compared to regular diesel. In addition to providing a renewable energy source to the transportation sector and reducing exhaust emissions, biodiesel may have the advantage of reducing the size and number of soot particles emitted. Thus, it is recommended that governments consider using blends of biodiesel in urban and commercial vehicles to enhance the quality of air.

Because of the findings of this study, the researchers recommend that policy makers include the variable emissions characteristics of biodiesel depending on biodiesel feedstock types in energy policies and environmental regulations in order to leverage the proper use of feedstock and biodiesel by manufacturer and consumers. Energy policies should be stipulated to encourage diesel manufacturers to come up with a proper selection of feedstock and blending ratios depending on region, season, and operating conditions. Environmental policies should provide consumers with guidelines on the selection of biodiesel types and blends to optimize both combustion efficiency and environmental sustainability. Agriculture departments should publish guidelines for farmers for growing environmentally friendly biodiesel feedstock.

### About the Authors

Ashok Kumar, PhD is Professor and Chairman of the Department of Civil Engineering and Dong-shik Kim, PhD is Associate Professor of Chemical and Environmental Engineering at The University of Toledo. Hamid Omidvarborna received his PhD in the summer of 2016; Manideep Yarlagadda, Sudheer Kumar Kuppili, and Nader Majed Sawtarie are Masters students at The University of Toledo.

### To Learn More

For more details about the study, download the full report at [transweb.sjsu.edu/project/1245.html](https://transweb.sjsu.edu/project/1245.html)