

Infrared-excitation for Improved Hydrocarbon Fuels' Combustion Efficiency - Concept and Demonstration

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ABSTRACT

This paper describes an innovative concept of using infrared (IR) excitation to help hydrocarbon fuels burn in internal combustion engines at a possible higher efficiency. In organic chemistry, hydrocarbons are known to be infrared-active and absorb photons in 3 - 20 μm wavelengths causing molecular vibrations that lower activation barrier and thus increase oxidation rate during combustion. As a result, IR-excited fuel becomes more combustible in engine, helping getting closer to the ideal of constant-volume combustion for higher cycle efficiency. Prototype IR-emitters were made from selective transition metal oxides with a spectral luminance in 3 - 16 μm wavelengths. The IR-excitation effect was demonstrated by testing at an engine lab of MTU (DaimlerChrysler Off-Highway) on its 8V4000M63 model heavy-duty diesel engine for marine applications, showing a 6 % reduction in fuel consumption. IR-excitation effect on flame structure was validated at Purdue University in a counterflow methane-air diffusion flame experiment, in which species concentrations for H_2 , O_2 , N_2 , CH_4 , CO , CO_2 , C_2H_2 , and C_2H_4 across the flame were measured using sampling and gas chromatography, while NO concentrations were measured using chemiluminescence analysis. The experimental results indicate the IR-excitation makes fuel burn faster and helps reduce fuel consumption by 6% and peak CO and NO emissions by about 15%. In addition, the results from an EPA FTP-75 test with the IR-emitters installed on a Ford F-350 light-duty diesel truck show a 5% improvement in fuel economy and about 38% reduction in both HC and CO emissions, while NOx and PM (particulate matter) emissions remain about the same, but the amount of SOF (soluble organic fraction) of diesel particulates emissions decrease by 10%. Though the preliminary tests seem to prove the concept, more evidences and works are required before a conclusion

on the efficacy of IR-excitation can be made and commercial value realized.

INTRODUCTION

Optimizing vehicle fuel efficiency today may require a combination of solutions including mass reduction, engine downsizing, and advanced powertrain technologies. Besides from the technology menu of fuel efficiency improvement that is pursued by automakers, this paper describes a simple retrofit technology that pretreats fuels with infrared (IR) excitation for better combustion efficiency without changing the engine specifications.

Using IR-excited fuels for improved fuel efficiency of internal combustion engines was first introduced in 2003 to an AFS (American Filtration Society) topical conference on reducing diesel and gas emissions by Wey [1]. IR technology is based on the fact that hydrocarbons are IR-active and absorb multi-photons in 3 - 16 μm wavelengths, causing molecular vibrations [2]. Photochemistry enhancement of reaction rates by reactant vibrational excitation have been demonstrated in laboratory dynamics studies [3]. These studies suggested exciting hydrocarbon fuels with infrared in aforementioned wavelengths could potentially improve combustion efficiencies. Even if that concept for better fuel conversion efficiency was scientifically predictable, a broadband IR-excitation source for the proposed applications did not commercially exist, until now.

Modifying the IR technologies used in Japan for agricultural applications since 1960's, we designed IR-ceramics from selective transition metal oxides that emit infrared in 3 - 16 μm wavelengths [4]. Transition metal oxides are used because of their unique property. The constituent electrons in transition metal oxide can be thermally agitated to reach a

neighboring higher energy level by absorbing ambient heat radiation, which exists at any temperature above Absolute Zero, or $-273\text{ }^{\circ}\text{C}$. When the excited electron returns to its initial state, it emits an IR photon in 3 - 16 μm wavelength range, depending on the variety of oxides used. As such, no additional energy source is required to power the IR-ceramics. The IR ceramic material is merely a thermal energy converter.

It is worth noting here that the proposed IR technology is not related to the unfounded magnet fuel saving technologies. According to photochemistry, the nuclear magnetic resonance (NMR) of magnetic nuclei in substance caused by applying magnetic field and short EM (electromagnetic) pulses is only in RF (radio frequency) range. Its energy, $e = h\nu$ in which h is Planck constant and frequency $\nu = 10^7$ Hz, is only one millionth ($1/10^6$) of the energy required to affect molecular structure at $e = h\nu$, with $\nu = 10^{13}$ Hz. There is no reason to believe a magnet device would improve fuel combustion. In contrast, the infrared in 3 - 16 μm wavelengths are in the frequency range of 10^{13} Hz, which provides the groundwork for this paper.

In the implementation for the proposed engine applications, the IR-emitting ceramics can be simply clamped to exterior of a nonmetal fuel supply line of the engine, because 3 - 16 μm wavelength photons can penetrate any nonmetal material. Hydrocarbons in the fuel traversing thorough the line will be exposed to infrared radiation and excited before the fuel enters cylinders for combustion. Thus, the IR-emitters may be retrofitted to any hydrocarbon-fuel powered engine, from the use of the simplest form of hydrocarbon (e.g. methane, propane) to a more complex hydrocarbons system (e.g. gasoline, diesels, and bio-diesels). Confirmatory test results demonstrating the IR-effect on reducing diesel engine emissions were reported in the 2005 AFS biannual topical conference by Wey [5]. Nevertheless, how IR-excitation participates in the thermochemical process of combustion to improve the fuels' conversion efficiency remained unidentified.

The combustion of multi-component commercial fuels (e.g. gasoline, diesels) in an engine involves many complicated processes, such as atomization, evaporation, turbulent mixing, and combustion timing. In the present study, to eliminate the complexities in a gasoline or diesel engine, the laminar non-premixed counterflow methane-air flame experimentation was used at Zucrow Laboratories, Purdue University (West Lafayette, IN) to investigate the IR-effect on the combustion of methane, which is the simplest form of hydrocarbon fuel. Counterflow flames are widely used in evaluation of chemical kinetic rates because they are one-dimensional and have a uniform strain rate [6]. It also allows the use of the software code developed by Sandia [7,8] to reveal chemical kinetics details with manageable

computational times. Besides, the methane mechanism and thermochemical database given in reference [9] can be used to predict and compare the measured concentrations of major species in the flame.

This paper starts with detailed descriptions on how infrared in 3 - 16 μm wavelengths may be absorbed by hydrocarbon molecules to affect their reaction rate during combustion, from a quantum mechanics view. A straightforward demonstration test was performed at an engine lab of MTU (DaimlerChrysler Off-Highway) by directly correlating the reduction of carbon dioxide (CO_2) concentration in the engine exhaust with the application of IR-excitation to the fuel. Additionally, the IR-excitation effect on combustion efficiency was investigated in a methane-air counterflow flame experiment at Purdue University. Lastly, an EPA FTP-75 test was performed on a Ford F-350 light-duty diesel truck to examine real world applications for the IR-excitation. Though the preliminary results in all these tests are very encouraging, there are numerous questions remain to be answered before a conclusion on total efficacy of the IR-excitation can be made.

THEORY

ABSORPTION OF INFRARED RADIATION

When a photon is absorbed by a molecule, it ceases to exist and its energy is transferred to the molecule in one of vibrational, rotational, electronic, and translational forms. Among them, the excitation of vibrational modes usually requires a photon with a wavelength typically shorter than 20 μm . In organic chemistry, hydrocarbon molecules are known to be IR-active and absorb photons in 3 - 16 μm wavelengths to cause molecular vibrations.

Some exemplary IR-excited vibrations in hydrocarbons are listed in Table 1. For example, the $\text{C}\equiv\text{C}$ bond in hydrocarbon molecule has a higher force constant than the $\text{C}=\text{C}$ bond so that the $\text{C}\equiv\text{C}$ bond absorbs IR at higher frequencies (i.e. higher energy) at $2100 - 2260\text{ cm}^{-1}$ (or $4.76 - 4.42\text{ }\mu\text{m}$ wavelengths) than the $\text{C}=\text{C}$ bond at $1650 - 1670\text{ cm}^{-1}$ ($6.06 - 5.99\text{ }\mu\text{m}$). It takes more energy to make the stronger $\text{C}\equiv\text{C}$ bond vibrate than it does to the $\text{C}=\text{C}$ bond. In practice, organic chemists have been using the IR absorption spectral information (so-called Infrared Correlation Charts) to identify unknown hydrocarbon specimens for decades [10].

MOLECULAR VIBRATIONS

It was recognized early in the study of chemical kinetics that increasing the energy of reactants increased reaction rate, and it was usually accomplished by simply raising the reaction temperature. However, in 1930's Evans and Polanyi illustrated the importance of molecular vibrational energy in

Table 1. IR absorption by hydrocarbon molecules.

ω (cm ⁻¹)	λ (μ m)	Bond Structure
1475	6.78-7.60	C-H (in alkanes)
2800-3000	3.33-3.57	C-H (in alkanes)
1450-1600	6.25-6.90	C=C bond in aromatic ring
1650-1670	5.99-6.06	C=C
2100-2260	4.42-4.76	C \equiv C
3000-3100	3.23-3.33	C-H (part of aromatic ring)
3300	3.03	C-H (C is acetylenic)
3020-3080	3.25-3.31	C-H (C is ethylenic)
1420-1470	6.80-7.04	Alkanes' -CH ₃
1375	7.27	Alkanes' -CH ₃
1430-1470	6.80-6.99	Alkanes' =C H ₂
1370, 1385	7.30, 7.22	Alkanes' -CH(CH ₃) ₂
1170	8.55	Alkanes' -CH(CH ₃) ₂
1370, 1395	7.30, 7.17	Alkanes' -C(CH ₃) ₃
910-920	10.87-10.99	*Alkenes' RCH=CH ₂
990-1000	10.00-10.10	*Alkenes' RCH=CH ₂
880-900	11.11-11.36	*Alkenes' R ₂ C=CH ₂
675-730	13.70-14.81	*Alkenes' RCH=CHR <i>cis</i>
965-975	10.26-10.36	*Alkenes' RCH=CHR <i>trans</i>
730-770	12.99-13.70	*Aromatic C-H ⁽¹⁾
735-770	12.99-13.61	*Aromatic C-H ⁽²⁾ <i>ortho</i>
690-710	14.08-14.49	*Aromatic C-H ⁽²⁾ <i>meta</i>
750-810	12.35-13.33	*Aromatic C-H ⁽²⁾ <i>meta</i>
810-840	12.35-11.90	*Aromatic C-H ⁽²⁾ <i>para</i>

* means "Out-of-Plane" ⁽¹⁾ Mono-substituted; ⁽²⁾ Distributed.

reaction dynamics [11]. Evans and Polanyi argued the reactant vibrational energy is the most effective at promoting reaction. Their expectation was that if the vibrational excitations were sufficient to lower the activation barrier of reactants, substantial rate enhancement would be realized. It is plausible from a standpoint of view of photoselective chemistry, which describes the influence of selective optical excitation on acquisition, storage and disposal of energy and on reactivity of molecules. Nonetheless, it was not until 1960's after the invention of lasers that scientists were able to use lasers to demonstrate increasing vibrational energy is indeed relatively more important in enhancing a molecular reaction than simply raising the reaction temperature.

Tunable lasers provide a very convenient method for obtaining selective vibrational excitations in molecules. A number of reactions of IR laser-excited species have been studied, in which the correlation between ground-state heats of reaction and vibrationally induced reaction rate enhancement is striking. Vibrational energy in some of these cases were found to enhance the reaction rate by two orders of magnitude [12]. It is concluded that chemical reactions can

be drastically enhanced by optical excitation from infrared lasers.

INFRARED MULTIPHOTON ABSORPTION AND EXCITATION

The molecular multiphoton process (MMP) has become an interesting research topic after the discovery that polyatomic molecules under collision-free conditions may absorb many infrared quanta from an IR laser. Based on the theoretical studies and available experimental information, a qualitative picture is drawn in Fig. 1 [13], which can be described as follows.

The molecular energy levels can be separated into three regions [14]. In the lowest energy range, region I (incoherent multiple photons interaction zone), the density of molecular states is very low and the IR field is interacting with isolated molecular states. In this region, multi-photon resonances are accounted for in terms of the molecular level-scheme of region I, so-called "ladder of vibrational states". After the molecule absorbs a few quanta, the density of molecular