



## Full Length Article

## Experimental and modeling study of farnesane



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## ABSTRACT

Several alternative synthetic fuels are in discussion as a replacement for conventional fuels like Jet A-1 to cope with limited supplies of crude oil as well as their emissions connected with its use such as the greenhouse gas CO<sub>2</sub>. One of the alternative fuels which have received high attention recently is farnesane (2,6,10-trimethyldodecane), a biofuel produced from sugar using a biotechnological process. In this paper, combustion characteristics of farnesane were investigated by measuring its ignition delay time using a shock tube at elevated pressure (16 bar) and two different stoichiometries ( $\varphi = 1.0$  and  $\varphi = 2.0$ ) and the laminar burning velocity at atmospheric and elevated pressures (1, 3, and 6 bar). These results were compared to a conventional Jet A-1 fuel showing that farnesane has a similar combustion behavior. Furthermore, a reaction model was developed capable to predict the measured combustion properties. The calculation of the ignition delay times yields excellent results when compared to the measurements; the computations of the laminar flame speeds are in good agreement with the measurements. In addition, the reaction model was analyzed to get further insight into the main reaction steps of farnesane oxidation.

## 1. Introduction

Until now crude oil is the dominant source of fuels for transportation. But the use of conventional transportation fuels is connected with at least two problems: They are produced from crude oil, which is an exhaustible raw material, and their combustion is connected with emissions such as the greenhouse gases CO<sub>2</sub> and water vapor (H<sub>2</sub>O). Further emissions are nitrogen oxides (NO<sub>x</sub>), and particulate matter [1–3].

Over the past years different liquid synthetic fuels were developed either based on other fossil resources, like Gas-to-Liquid fuels (GtL) made from natural gas, Coal-to-Liquid fuels (CtL) from coal [4–6], or obtained from biomass (BtL). Typical organic raw materials are sugar, vegetable oils, and fatty acids but also wood-based biomass [1,2,7,8]. At present, alternative aviation fuels are predominantly developed as drop-in-fuels because of the long lifetimes of jet engines and due to stricter regulations [1]. In general, conventional jet fuel has to comply with the standard ASTM D1655 and synthetic jet fuel with ASTM D7566 [2,8] ensuring that the combustion is reliable and safe under all flight conditions, e.g. cold temperatures at high altitude. Moreover, this certification assures that the new synthetic jet fuel is compatible with current engines and technology and that synthetic jet fuel blends are interchangeable with conventional aviation fuels to prevent any

logistics or storage problems at airports that may arise due to the handling of different fuels.

The use of coal or natural gas as feedstock for synthetic fuel production via the Fischer-Tropsch process (CtL or GtL) led to the first approved alternative fuels for blending up to 50%. Moreover a CtL production process exists which yields a fully synthetic jet fuel (FSJF), meaning that it can be used as a replacement of crude oil based fuels without blending [2]. This is of course an alternative to the use of crude oil, but it is neither sustainable nor can a reduction of CO<sub>2</sub>-emissions be expected. However, Fischer-Tropsch technology also allows the use of biomass as raw material to produce synthetic fuels; but to our knowledge up to now no commercial or large scale plant is operational using this technology.

To benefit from biofuels – a sustainable replacement for crude oil based fuels, reduction of overall emissions, including the greenhouse gas CO<sub>2</sub> [3,9] – other fuels, processes and technologies were developed. Approved in 2014 [10], a biofuel for aviation which can be used as a drop-in-fuel is farnesane [8], a branched alkane with 15 carbon atoms as it is shown in Fig. 1. Its chemical name is 2,6,10-trimethyldodecane; for a better readability, only the name farnesane is used in this paper. The production of farnesane has three major steps. At first, sugar is fermented by yeast to farnesene, a molecule with four double bonds [11]. The second step is the hydrogenation from farnesene to farnesane

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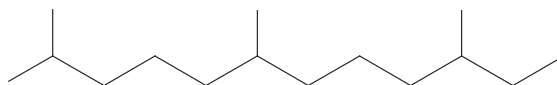


Fig. 1. Chemical structure of the farnesane molecule (2,6,10-trimethyldodecane),  $C_{15}H_{32}$ .

Table 1

Selected physical properties of farnesane and the specific Jet A-1 used in this study (data of farnesane are taken from Ref. [8], formula of Jet A-1 are empirically determined from its H/C ratio of 1.9).

	Farnesane	Jet A-1 [22]
Formula	$C_{15}H_{32}$	$C_{12}H_{23}$
Molar mass (g/mol)	212.41	167
Density at 288 K ( $g/cm^3$ )	0.7731	0.8035
Boiling temperature (K)	520	423–551
Flashpoint (K)	380.65	313.15
Viscosity at 253 K ( $mm^2/s$ )	14.13	4.122

which in the last step is purified by distillation [8]. Whereas Jet A-1 is a multicomponent mixture [2] farnesane is a single component with a molecular size being in the upper range of the molecular size distribution typically found in Jet A-1. Since it is a pure component only some physical properties (selected properties are shown in Table 1) are in the acceptable range for aviation fuels like boiling point or flashpoint. Density and viscosity are out of the range [8], so consequently farnesane is approved as a blending component to Jet A-1 up to an amount of 10% only. For comparison, HEFA (hydrotreated esters and fatty acids) kerosene, a biofuel made from vegetable oils consisting of different, predominantly branched alkanes, is approved as a drop-in-fuel up to 50% [8]. Passenger flights from Florida to Sao Paulo [12,13] and in Germany [13,14] were already operated using a 10% farnesane blend as jet fuel as well as a delivery flight of an Airbus A350 from Toulouse to Hong Kong [15].

Since farnesane is not only considered as a biofuel for aviation but also as an alternative for diesel fuel [16], few studies have focused on the ignition and decomposition behavior [16–19]. Moreover, engine emissions tests were performed with jet fuel [3,8] as well as diesel blends [20]. Recently speciation data for farnesane were published [21] providing information on its reaction behavior and product distribution.

The aim of the current paper is to present new experimental data for two major combustion properties, ignition delay time and laminar burning velocity, as well as a first reaction model developed to describe the combustion of farnesane; the model's performance with respect to the experimentally measured combustion properties will be discussed.

## 2. Experimental study

Two global combustion properties of farnesane were investigated: the ignition delay time and the laminar burning velocity. The obtained results were compared to measurements of a conventional Jet A-1 fuel. An overview about selected physical properties of farnesane as well as of the specific Jet A-1 used in the experiments is given in Table 1.

### 2.1. Ignition delay time

#### 2.1.1. Experimental setup

The experiments were carried out in a high pressure shock tube with an internal diameter of 46 mm. It was divided by aluminium diaphragms into a driver section of about 10 m and a driven section of 3.25 m in length. The driver section was heated to 393 K and loaded with mixtures of helium and argon controlled by Bronkhorst mass flow controllers to achieve tailored interface conditions [23]. The driven section was heated to 453 K and pumped down to pressures below

$10^{-4}$  mbar by a turbomolecular pump. Gas mixtures were prepared in a 5 L stainless steel storage vessel, which was heated to 180 °C, nitrogen flushed and evacuated using a separate rotary vane pump to obtain pressures below  $10^{-2}$  mbar. For each experiment a new mixture was prepared by injecting the liquid fuel with a syringe onto fibers permanently purged by hot nitrogen which evaporated and transported the fuel into the evacuated vessel. Preheated synthetic air (80 vol-%  $N_2$ , 20 vol-%  $O_2$ ) and nitrogen were added thereafter adjusting equivalence ratio and dilution. All gases were delivered by Linde at purities of  $N_2$ : 99.999%, syn. air: 99.9995%. After a mixing time of 10 min the fuel-air- $N_2$  mixture was filled into the shock tube. The optimal mixing period, gas preheat temperatures, and the mixtures' composition were determined and controlled by gas chromatographic analysis monitoring fuel degradation and recovery rate.

The incident shock speed was measured over three 30 mm intervals using four piezo-electric pressure gauges. The temperature and pressure behind the reflected shock wave were computed from the measured incident shock speed and the attenuation using a one-dimensional shock model. For farnesane the thermodynamic data by [24] were used and for Jet A-1 the data of Jet A (g) given by Goos et al. [25]. The concentration of Jet A-1 (g) was calculated using its average composition ( $C_{12}H_{23}$ ) and the equivalence ratio of the experiment. The estimated uncertainty in the reflected shock temperature is less than  $\pm 15$  K throughout the temperature range of our measurements.

The ignition was observed by measuring pressure profiles with piezo-electric gauges (PCB® 112A22 and Kistler® 603B coated with a thin layer of RTV106 high temperature silicone rubber) located at a distance of 1 cm from the end flange. In addition, the  $CH^*$ -emission at 431 nm, at the same position and through the end flange as well, was selected by a narrow band pass filters (Hugo Anders, FWHM = 5 nm) and measured with a HAMAMATSU® R3896 photomultiplier in combination with a FEMTO® HLVA-100 logarithmic amplifier. Moreover, two measurement ports at a distance of 7 cm and 10 cm from the end plate were detecting the  $CH^*$ -chemiluminescence emitted by the propagating deflagration wave. All ignition delay time values shown in this paper were determined by measuring the time difference between the initiation of the system by the reflected shock wave at the end flange and the occurrence of the maximum of the  $CH^*$ -signal at the side on measurement port 1 cm away from the end plate; this characteristic can be reproduced easily from the corresponding simulations. The experimental setup allows measurements of ignition delay times up to 10 ms depending on the temperature. Post-shock compression effects mainly due to the interaction of incident gas with the attenuated reflected shock wave introduce a time dependent pressure increase  $p = p(t)$  with a maximum compression of  $p_5/p_5(t=0) = 1.22$  at about 8 ms resulting in a temperature increase  $T = T(t)$  and thus, in an acceleration of the reactive system towards ignition.

#### 2.1.2. Experimental ignition delay time determination

The ignition delay times of farnesane and Jet A-1 were determined at stoichiometric ( $\varphi = 1.0$ ) and fuel-rich ( $\varphi = 2.0$ ) conditions. The fuel-synthetic air mixtures were diluted with nitrogen (50% mixture/50%  $N_2$ , defined as dilution 1:2). The temperature range was  $800 K \leq T \leq 1400 K$  at initial pressures of about 16 bar. A pressure profile as well as radial and axial  $CH^*$ -emission profiles of a single experiment are presented in Fig. 2: The pressure signal of the farnesane- $O_2$ - $N_2$  mixture ( $\varphi = 1.0$ , dilution 1:2) at an initial temperature  $T_i = 883 K$  and an initial pressure  $p_i = 16.85$  bar (green curve) shows at the very first stage a two-step increase due to the incident and reflected shock wave; this is followed by: (i) a slow pressure increase due to gas dynamic effects as described above without any influence of the fuel's combustion; (ii) a turning point at 2500  $\mu s$  due to the reflected shock wave passing the contact surface; and (iii) a further increase due to the superposition of gas dynamic effects, caused by the propagation of the reflected shock wave into the driver gas, and the heat release by the ignition. Pressure profiles from experiments without ignition or from

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