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ABSTRACT

In the present work, Hexanol a biofuel produced from agro-waste is examined as a potential alternative to fossil fuel. A single-cylinder water-cooled Diesel engine was used for the tests. The mechanical injector was replaced with a solenoid injector and provisions were made for mounting an injector in the inlet port. Diesel was injected in-cylinder during the late compression stroke and hexanol was injected into the inlet port of the engine. The engine was operated at rated load and the ratio of hexanol to Diesel was varied. The tests were carried out at injection pressures (P_{inj}) of 400, 500, and 600 bar. Combustion and emission data were collected and compared to that of neat Diesel combustion. Increased peak pressure and heat release rates were observed. Oxides of nitrogen together with smoke emissions decreased, with an increasing percentage of hexanol at each P_{ini} . There was a marginal increase in indicated thermal efficiency even though the heating value of hexanol is lower. This study suggests hexanol could be utilized as an alternative fuel in advanced reactivity controlled compression ignition (RCCI) combustion.

1. Introduction

Global air pollution is estimated to reduce people's life expectancy by 1.75 years. In the year 2017, 92% of the population lived in areas that exceeded particulate matter emissions ($PM_{2.5}$) norms set by the World Health Organization [\[1\]](#page-7-0). India has 15 of the 20 most polluted cities in the world [\[2\]](#page-7-0). As of 2018, 25.1 million commercial vehicles are out there in the world and 16% of the world's $CO₂$ emissions are based on road transport [\[3\]](#page-7-0). The measures to reduce global air pollution and its detrimental effects on the environment include after-treatment devices, electrification, and advanced engine technologies. After-treatment devices are widely preferred because minimal engine modifications are required. However, adding multiple devices on the tailpipe will cause additional fuel penalties and increases vehicle costs [\[4\]](#page-7-0). On the contrary, electrification has inherent benefits. Yet, complexities associated with electrical power supply, storage in batteries, and charging infrastructure delay its immediate large-scale implementation [\[5\].](#page-7-0) Therefore, a suitable solution is innovations in advanced combustion technologies to cut down emissions and subsequent deterioration of the environment.

Most of the commercial heavy-duty (HD) vehicles employ internal combustion engines with Diesel as their primary fuel. Though gasoline engines produce less particulate matter and NO_X when compared to Diesel engines [\[6\],](#page-7-0) the Diesel engine is predominantly used because of its high thermal efficiency and fuel economy [\[7\]](#page-7-0). The major problem

with Diesel engines is its inherent NOx and soot trade-off which is a barrier against the concurrent reduction of these pollutants [\[8\].](#page-7-0) The trade-off can be attributed to the heterogeneous nature of combustion. This could be avoided by operating the engine in homogenous charge compression ignition (HCCI) mode but drawbacks of limited operating range and combustion control creep in [\[9\]](#page-7-0).

Several combustion strategies emerged since the beginning of this century that aimed at premixed combustion of Diesel like fuels i.e. HCCI, partially premixed combustion (PPC), premixed low-temperature combustion (LTC), reactivity controlled compression ignition (RCCI) [\[10\].](#page-7-0) In premixed LTC, the low-temperature combustion reduces the formation of NOx and the premixed combustion curtails the production of soot species from the engine [\[11\].](#page-7-0) In the RCCI concept, the ignition qualities of two different fuels are utilized extensively so that premixed LTC could be attained. RCCI mode is advantageous with regard to combustion control and extended load operations which are lacking in the HCCI mode [\[12\].](#page-7-0) The increase in thermal efficiency linked with premixed LTC can be attributed to reduced heat transfer losses and the avoidance of high-temperature gradients in the cylinder [\[13\]](#page-7-0).

In RCCI, two fuels; one with good ignition quality (higher cetane index) termed as high reactive fuel (HRF) and the other with lower ignition quality (lower cetane index) termed as low reactive fuel (LRF) are used. M. Bharathiraja et al. [\[14\]](#page-7-0), performed exergy analysis on gasoline fumigated Diesel engines and found out that fumigation of gasoline replaces the amount of direct-injected Diesel with a reduction

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in both NO_X and soot emissions. At full load, the increment in brake thermal efficiency (BTE) added up to 3.8% accompanied by an increase in carbon monoxide (CO) and unburnt hydrocarbon (UBHC) emissions to 5 folds and 4 folds respectively. The increase in BTE was attributed to the higher latent heat of vaporization of gasoline which reduces the incylinder temperature and therefore increases volumetric efficiency in addition to the improved combustion because of the homogenous mixture formed by fumigated gasoline. Pandian and Anand [\[15\]](#page-7-0) attained a maximum thermal efficiency increase of 14%. They compared the emissions with compression ratios of 17.5 and 15 and found that NO_X and smoke were less than 0.5 g/kWh and 0.02 FSN at both compression ratios respectively. With a reduced compression ratio, CO emission reduced, whereas HC emissions were reported to increase.

The use of renewable fuel in RCCI is gaining widespread attention, due to its carbon neutrality with a substantial reduction in $\rm NO_{X}$ and soot [\[16\]](#page-7-0). Utilization of first-generation bio-alcohols like methanol, ethanol (lower alcohols) in engine applications dates back to several decades

[\[17,18\].](#page-7-0) Ethanol and methanol find their applications predominantly in spark-ignition engines where it is usually utilized as blends with gasoline [\[19,20\].](#page-7-0) The presence of OH group in alcohol fuels enhances soot oxidation in diffusion combustion and lowers the formation of soot species from the engine [\[21\].](#page-7-0) The use of lower alcohols (less than 3 carbon atoms) in compression ignition engines is restricted owing to low cetane index, lower heating value, and corrosiveness due to fuel bound oxygen [\[22\].](#page-7-0) Usman Asad et al. [\[23\],](#page-7-0) achieved dual-fuel LTC with ethanol and Diesel over the entire load range from 3.9 to 18.2 bar with low NO_X and soot, while retaining Diesel like efficiencies. NO_X reduction was obtained with a trade-off of reduced combustion efficiency and stability. Yaopeng Li et al. [\[24\],](#page-7-0) worked on the optimization of methanol Diesel RCCI combustion and stated the importance of EGR percentage and intake air temperature on combustion stability and control. Methanol of 66.5% was observed to be optimal in terms of lower fuel consumption and emissions.

First-generation biofuels have drawbacks as it competes with the

Clostridium carboxidivorans

Fig. 1. Waste to Fuel: Production of hexanol.

food supplies. Second-generation biofuels involve the conversion of waste biomass or waste *syn*-gas from industries into fuels [\[25\].](#page-7-0) John Phillips et al. [\[26\],](#page-7-0) produced higher alcohols like butanol, hexanol from syngas with *Clostridium carboxidivorans* bacterium which is also an economical process. Syngas is a mixture of CO, $H₂$ and CO₂ and is a manufacturing waste gas obtained excessively from steel plants ([Fig. 1](#page-1-0)). Zhang K. et al. [\[27\]](#page-7-0), proposed a synthetic way of enhanced production of 1-hexanol from glucose with the help of *E. coli* bacterium that optimizes the biosynthesis production mechanism.

The long-chained alcohols with carbon (C) atoms greater than 3 and possessing high molecular weight are termed as higher alcohols [\[28\]](#page-7-0). With the increase in C atoms in the alcohol, the heating value and the cetane index increase, which makes alcohol with high carbon content a better choice in terms of improved ignition qualities [\[29\]](#page-7-0). Additional benefits include complete blending with Diesel and no phase separation.

Babu and Anand [\[30\],](#page-7-0) prepared a blend of biodiesel and Diesel with hexanol and pentanol and analyzed the engine performance and emissions. The maximum BTE obtained was close to 31% in the blend of biodiesel (90%), Diesel (5%), and hexanol (5%). The UBHC, CO, NO_X , and smoke were less in all the blends when compared with neat Diesel operation. Pandian et al. [\[31\],](#page-7-0) blended hexanol with biodiesel in substitution ratios of 10 and 20 percentages by volume respectively and stated that the BSFC reduces with increasing percentages of hexanol replacement in biodiesel. They reported an overall decrease in smoke, HC and CO emissions while comparing with neat Diesel or neat biodiesel operations. Neat biodiesel operation was characterized by 4.71% increase in NO_X when compared to neat Diesel operation. However, by adding 10% and 20% of hexanol to biodiesel, NO_X emissions dropped by 3.1% and 4.7% respectively. Mohamed Nour et al. [\[21\]](#page-7-0), blended heptanol and octanol with Diesel in 10% and 20% blend ratios respectively and observed an overall reduction in NO_X and soot, but a hike in HC and CO emissions. The peak heat release and maximum combustion efficiency were observed in the case of 20% heptanol blend with Diesel. Ashok et al. [\[32\],](#page-7-0) blended octanol and biodiesel and used the mixture in a Diesel engine. An increase in thermal efficiency was observed up to 30% blending of octanol with biodiesel. Combustion was characterized by longer ignition delay and predominant premixed combustion resulting in a high rate of pressure rise. All these studies focus on using higher alcohol as a blend with Diesel or biodiesel. Implementation of hexanol as LRF in a RCCI regime is a novel approach and has not been attempted at the time of this work.

The present work encompasses the scope of replacing petroleumbased fuels with renewable biofuels like hexanol wherein waste from food and agro-industry is converted into a potential energy source.

In the present study, Hexanol and Diesel were used as LRF and HRF respectively, in a RCCI engine. A modified single-cylinder water-cooled engine was used for the investigation. Provisions were made for direct injection of Diesel at 400, 500, and 600 bar injection pressure (P_{ini}) and manifold injection of hexanol at 3 bar P_{ini}. Experiments were carried out at rated load and the proportion of hexanol to Diesel was varied. Combustion and emission data were recorded and plotted against that of neat Diesel to investigate the influence of injection pressure and the proportion of hexanol to Diesel on engine combustion. Implementation of exhaust gas recirculation and multiple injections as well as incorporation in a multi-cylinder engine are the future scopes of the work.

2. Methodology

The study is intended to examine the utilization of hexanol as a substitute for petroleum-based gasoline. Its effect on combustion, performance, and emission in a single-cylinder modified Diesel engine operating in RCCI mode is explored. Hexanol has a lower cetane index compared to Diesel [\(Table 5](#page-3-0)) and therefore is used as LRF along with Diesel which is the HRF. Hexanol is inducted during early suction stroke whereas Diesel is directly injected during the late compression stroke. A common-rail along with electronically controlled solenoid injector is

used to inject Diesel at higher P_{inj} of 400, 500, and 600 bar in-cylinder in contrast to manifold injection of hexanol at 3 bar P_{ini} . The engine was operated at rated load and the proportion of LRF to HRF was varied from 40:60 to 60:40. Replacement above 60% was not done because of the limitation of the flow rate of the port injector. The tests were repeated for 400, 500, and 600 bar P_{inj} and data were collected for engine performance and emissions study. The engine operating conditions are shown in Table 1.

3. Experimental setup

A modified Kirloskar AV1 water-cooled DI engine was used in the investigation. [Table 2](#page-3-0) presents the technical specifications of the test engine. The mechanical fuel injection system was replaced with a Bosch make high-pressure common rail direct injection (CRDi) system which consists of a high-pressure pump, common rail, and electronically controlled solenoid injector for direct injection. Arrangements were made on the cylinder head to incorporate a port injector. A Denso make injector was utilized for manifold injection of fuel at low pressure. National Instruments (NI) make open electronic engine control unit (EECU) was used for engine control. The CRDi injector as well as the port injector were connected to the EECU using NI direct injection driver system (DIDS) software. The rail pressure and engine speed were maintained using PID control. Intake air to the engine was heated using an air preheater in the inlet. Gravimetric measurement of fuel flow rate was done using regularly calibrated electronic weighing scales. Sensors and transducers were used for gauging and monitoring operating parameters as well as the engine combustion. AVL Digas analyzer and AVL 437c were used to measure the emissions and smoke opacity respectively. [Fig. 2](#page-3-0) shows the schematic diagram of the engine. The measuring range and accuracy of the instruments are given in [Table 3](#page-3-0) and the uncertainty in measurement is shown in [Table 4](#page-3-0).

Test Fuels: Hexanol fuel used in this investigation was procured from Research-Lab Chemical Corporation, Mumbai, India. Diesel was purchased from a local filling station in Chennai, India. The properties of the test fuel are summarized in [Table 5](#page-3-0).

4. Results and discussion

4.1. In-cylinder pressure and rate of heat release

In-cylinder pressure (P_{cyl}) is a measurable parameter that helps to understand the combustion process inside the combustion chamber, which is otherwise difficult to perceive. It comprises of both compression pressure as well as combustion pressure. The P_{cyl} is plotted against crank angles at different P_{inj} for various fuel combinations in [Fig. 3](#page-4-0). It is observed from [Fig. 3\(](#page-4-0)a), (b) and (c) that with increasing P_{inj} the incylinder pressure advances for all the fuel combinations. The peak pressure (P_{max}) also increases with increasing P_{ini} . This is attributed to the fact that with increasing P_{inj} , the fuel droplets break down into finer

Table 2

Technical specifications of the test engine.

Table 3

Measurement device range and accuracy.

spray therefore easier vaporization and better combustion. It is also observed from [Fig. 3](#page-4-0)(a), (b) and (c) that, with an increasing proportion of hexanol, the Pmax increases owing to improved combustion due to oxygenated fuel. The pressure curve also advances with the increasing proportion of hexanol owing to reduced ignition delay as observed from [Fig. 4\(](#page-5-0)d).

The heat release rate (HRR) shows how effectively the chemical energy of the fuel is transformed into heat energy. HRR is derived from pressure-crank angle data by differentiation. [Fig. 3\(](#page-4-0)a), (b), and (c) show the HRR on the right-side axis for different fuel combinations at P_{inj} of 400, 500, and 600 bar. It is observed that for all the fuel combinations peak of HRR (HRR_{max}) increases with increasing P_{inj} which shows better

combustion which is attributed to better atomization and mixing. It also advances in terms of crank angle and increases in amplitude with an increasing percentage of hexanol as in the case of the pressure curve, owing to improved combustion as a result of oxygenated fuel. It is noticed that at 600 bar P_{inj} the HRR of Diesel is comparable to that of DH combinations which goes on to show that higher P_{inj} improves the combustion irrespective of the fuel.

4.2. Combustion parameters

Start of Combustion (SOC) is termed as the point at which about 5% of the fuel has undergone combustion. In this work, SOC is calculated as the crank angle at which the HRR curve passes from negative to the positive y-axis [\(Fig. 3](#page-4-0)). SOC for Diesel hexanol (DH) combinations is compared with that of Diesel for different P_{inj} in [Fig. 4\(](#page-5-0)a). It is observed

Table 5

Test Fuel Properties.

Fig. 2. Schematic diagram of the test engine.

Fig. 3. P_{cyl} vs. crank angle and HRR vs crank angle at P_{inj} of (a) 400 bar (b) 500 bar (c) 600 bar for different fuel combinations.

that at all P_{inj}, SOC for DH combinations is advanced compared to Diesel. This is because of the early induction of hexanol during suction stroke which results in the formation of a homogenous mixture ready for combustion by the time Diesel is injected. It can be observed from [Fig. 4](#page-5-0) (a) that with an increasing proportion of hexanol, SOC further advances owing to an increased premixed (homogenous) fraction. It is also observed that with an increase in Pinj from 400 to 600 bar, the SOC advances, owing to improved atomization and therefore easier mixture formation and lower ignition delay [\(Fig. 4](#page-5-0)(d)).

End of Combustion (EOC) is defined as the crank angle at which 90% of the fuel has undergone combustion. In this study, EOC has been computed based on mass fraction burnt. [Fig. 4](#page-5-0)(b) shows EOC for the different fuel combinations at different P_{inj} compared to that of Diesel. At 400 and 500 bar P_{inj} it is observed that the EOC is delayed for DH combinations than Diesel. This is credited to the increased quantity of fuel injected to compensate for the lower heating value of the DH combination. The EOC of all the DH combinations is similar. With increasing Pinj, EOC remains unaffected except in the case of Diesel where it extends. This could be attributed to the shorter premixed combustion phase and increased diffusion combustion as a result of better atomization and mixing with increasing injection pressure.

Combustion duration (CD) is the interval between SOC and EOC. The CD for different fuel combinations at different P_{ini} is plotted in [Fig. 4\(](#page-5-0)c). CD for DH combinations is higher than Diesel as a result of advanced SOC and extended EOC as observed in [Fig. 4](#page-5-0)(a) and (b). With an increasing percentage of hexanol, there is a marginal surge in CD at 600 bar whereas at 400 and 500 bars, the change is insignificant. The increase in CD with an increasing proportion of hexanol could be attributed to the lower heating value of DH combinations.

Ignition Delay (ID) is an important property as it affects the combustion inside the cylinder. It is the time between the start of injection (SOI) and SOC. Longer ID could lead to the accumulation of fuel in the cylinder during premixed combustion which could lead to increased incylinder temperature and therefore higher NOx emissions. ID for the DH fuel combinations is compared and plotted against that of Diesel for different P_{inj} in [Fig. 4\(](#page-5-0)d). It is observed that with increasing P_{inj}, ID decreases, due to better atomization and therefore quicker evaporation, and hence more effective mixture formation at higher P_{inj}. Another observation is the decrease in ID with an increasing proportion of hexanol for all Pinj. This is because of the increased quantity of hexanol-air mixture available for combustion as hexanol is inducted earlier and a homogenous mixture with air is formed by SOI.

4.3. Emissions

Exhaust emissions play a vital role in engine combustion research and the selection of alternative fuel. These emissions depend on the physical, chemical properties of the fuel and the in-cylinder conditions. The major tailpipe emissions include CO, HC, NOx, and smoke. Out of these NOx and smoke are difficult and expensive to control. The present study aims at the concurrent reduction of these two. [Fig. 5](#page-6-0) depicts the comparison of different emissions for DH combinations at different P_{ini}.

Fig. 4. SOC, EOC, CD, ID for DH combinations compared to Diesel.

CO emissions are plotted for DH combinations against P_{inj} of 400, 500, and 600 bar in [Fig. 5](#page-6-0)(a). It can be noticed that with increasing P_{ini} , CO emissions decrease, due to better atomization and therefore better mixing and oxidation with increased Pinj. The CO emissions for DH combinations initially increase, and then decrease with an increasing proportion of hexanol. This could be because of better oxidation of CO to $CO₂$ in the presence of excess oxygen. At lower P_{ini} the CO emissions for DH are less than Diesel whereas at higher P_{inj} Diesel shows lower CO emissions.

Un-burnt hydrocarbon emissions for DH combinations are compared to those of Diesel in [Fig. 5\(](#page-6-0)b). It is observed that for Diesel, the HC emissions decrease with increasing P_{ini} in the pressure range of 400–600 bar. This is a result of better atomization leading to better mixing and combustion. In the case of DH combinations, there is an increase in HC emissions with increasing P_{ini}. This is due to increased diffusion combustion as can be observed in [Fig. 3](#page-4-0). The lower cetane index of hexanol in contrast to Diesel depreciates the auto-ignition property and promotes the quenching effect in lean regions leading to increased HC emissions. In addition, the cooling effect of hexanol owing to the higher latent heat of vaporization aids in increased HC emissions. The effect of fuel bound oxygen is opposed by these two factors. As a result, the HC emissions increase with the increasing proportion of hexanol.

NO emissions are plotted for DH combinations and compared to Diesel at P_{inj} of 400, 500, and 600 bar in [Fig. 5](#page-6-0)(c). It is observed that with an increase in Pinj, NO emissions increase for both Diesel and DH combinations owing to improved atomization and improved combustion

which leads to increased in-cylinder temperature. At all P_{inj}, it is observed that the NO emissions for DH combinations is less than that of Diesel owing to LTC as well as lower heating value of hexanol compared to Diesel. With the increasing proportion of hexanol in DH combinations, the NO emissions further reduce owing to lower in-cylinder temperature-induced due to the cooling effect of hexanol and its lower heating value.

Typically, there is a tradeoff between NO and smoke emissions, i.e. if NO decreases, smoke increases. [Fig. 5](#page-6-0)(d) depicts the smoke opacity for DH combinations compared to Diesel fuel at different P_{ini} . It can be observed from [Fig. 5](#page-6-0)(c) and (d) that there is a simultaneous reduction of NO and smoke in the case of DH combinations. With an increase in P_{ini} from 400 to 600 bar, it is observed that the smoke emissions reduce for both Diesel and DH combination owing to improved atomization leading to better oxidation at higher P_{ini} . With an increasing proportion of hexanol in DH combination, smoke emissions further decrease. This is because, with an increasing proportion of hexanol, more amount of homogenous mixture is ready for combustion at the time of direct injection. Therefore there are reduced fuel-rich zones and hence lower smoke emissions as observed in [Fig. 5\(](#page-6-0)d).

4.4. Efficiency

The efficiency of an engine is well-defined as the ratio of work done by the engine to the heat energy delivered to it. In an IC engine, the heat energy is supplied by the chemical energy of the fuel. The chemical

Fig. 5. Exhaust emissions for DH combinations compared to Diesel.

energy of the fuel is transformed into heat energy during combustion and the combustion gases exert pressure on the piston thereby doing mechanical work. The indicated thermal efficiency (η_{ith}) takes into consideration the indicated power rather than brake power for

Fig. 6. Indicated thermal efficiency for DH combinations compared to Diesel at different P_{inj}.

calculation. The η_{ith} at rated load for DH combinations is plotted and compared with Diesel at different P_{inj} in Fig. 6.

As observed from the figure, with an increase in P_{ini} there is a marginal rise in the η_{ith} for both Diesel and DH combinations. This increase in η_{ith} is attributed to improved combustion owing to improved atomization at increased P_{ini} . It is apparent that η_{ith} increased marginally for hexanol blends at all P_{ini} . The increase in η_{ith} is attributed to oxygenated hexanol which aids the combustion. However, with a further increase in the proportion of hexanol beyond 50%, it is observed that η_{ith} reduces. This is because the increase in efficiency owing to the oxidation effect of hexanol is countered by the lower heating value of hexanol. It can be inferred from Fig. 6, that DH 40 gives the best η_{ith} at 600 bar P_{ini} .

5. Conclusion

1-Hexanol was investigated as an alternative to petroleum-based fuel in a single-cylinder Diesel engine in dual-fuel mode. The objective being the concurrent reduction of smoke and NO of Diesel engine by the implementation of RCCI and using renewable fuel derived from agricultural waste. Being renewable and produced from agro-waste, hexanol would improve the farmer's economy. The engine was tested with Diesel (in-cylinder) and hexanol (port) in different proportions at direct P_{ini} of 400, 500, and 600 bar and rated load. The combustion, emission, performance data were acquired for Diesel and hexanol combinations in RCCI mode and the results were compared to Diesel operation. The following conclusions are made from the investigation:

- (a) P_{max} and HRR_{max} increased and advanced with the increasing proportion of hexanol. At lower Pinj (400, 500 bar), both P_{max} and HRR_{max} are higher than that in the case of Diesel, even with a lower heating value of hexanol which shows improved combustion. At 600 bar P_{ini} , the P_{max} and HRR_{max} for DH and Diesel are comparable.
- (b) ID decreases with an increasing proportion of hexanol for all P_{ini} , which results in advanced SOC. The extended diffusion combustion phase leads to an extended CD as well.
- (c) Simultaneous reduction of smoke and NO is attained for DH combinations at all P_{inj} , without the use of EGR. There is an increase in HC and CO emissions which is typical of LTC combustion. Considering exhaust emissions, 500 bar P_{ini} and 60% proportion of hexanol gives the lowest emissions.
- (d) There is a marginal increase in η_{ith} at rated load for DH combinations (40%, 50% hexanol). P_{inj} of 600 bar and hexanol proportion of 40% gives the best η_{ith} . With a further increase in the proportion of hexanol, η_{ith} decreases.

It can be concluded from the study that hexanol is a potential alternative to petroleum fuel. Though there is a hurdle in the form of fuel costs, it could be overcome by setting up production plants where hexanol could be produced in bulk. With bulk production, the current cost of hexanol (\sim 5\$) could be brought down on par with Diesel fuel (\sim 1\$). The increased fuel cost is a trade-off to be made for lower emissions. Hexanol with Diesel fuel in dual-fuel mode gives reduced emissions and increased indicated thermal efficiency. The emission could be further reduced employing EGR and multiple injection techniques. This is the future scope of the work.

CRediT authorship contribution statement

Justin Jacob Thomas: Conceptualization, Validation, Writing original draft. **V.R. Sabu:** Resources, Writing - review & editing. **G. Basrin:** Methodology, Software, Formal analysis. **G. Nagarajan:** Writing - review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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