NUMERICAL ANALYSIS OF DETONATION STABILITY IN A ROTATING DETONATION ENGINE FUELLED WITH BIOGAS AND HYDROGEN

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DEDICATION

This thesis is dedicated to my mother, my greatest supporter and pillar in my life, who taught me that the finest kind of knowledge to have is knowledge gained for the benefit of others.

To my father, who ingrained in me the belief that hard work pays off.

To Amaleen, who has been a strong emotional supporter throughout my doctoral study and has also assisted me in becoming the best version of myself.

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ABSTRACT

The novel rotating detonation engine (RDE) fuelled with biogas offers a significant contribution to the application of combustion engines powered by renewable-based fuels. However, the potential of a biogas-fuelled RDE has never been properly examined in terms of key operating parameters such as ignition intensity, equivalence ratio, and total mass flow rate (MFR). Hence, the primary research goal for the current numerical study was to examine the stability of continuous rotating detonation waves (CRDW) in RDEs powered by hydrogen and biogas on the basis of the aforementioned operating parameters. The numerical model of CRDW was first established to represent the CRDW stability. Following that, the modified one-step chemistry for biogas detonation was developed and merged with the validated CRDW numerical model. The impact of the above-mentioned critical operating parameters on CRDW stability in the biogas-fuelled RDE was explored using the validated CRDW numerical model, which was merged with the modified one-step chemistry for biogas detonation. The CRDW numerical model revealed that the predicted CRDW pressure was within 10% of the experimental data. The one-step model was compared to experimental data and the detailed chemistry data, revealing 15.75% and 8.29% discrepancies in biogas detonation velocities. The result is that in a fuel-lean non-premixed environment at fixed ignition intensities, the biogas-fuelled RDE outperformed the hydrogen counterpart in terms of detonation stability, with the predicted time to achieve a stable one-wave CRDW in the former RDE being 1327 microseconds shorter than that of the latter RDE. However, the former RDE fell short in detonation sustainability, as predicted by the wave longevity. After 0.0146 seconds from the one-wave emergence, the CRDW was extinguished in the former RDE, while the CRDW pressure was only decreased by 1.52% in the latter RDE. The fundamental explanation for this was that biogas, which has lower diffusivity and reactivity than hydrogen, created an imbalance in counter-rotating waves, resulting in a faster CRDW mode transition than hydrogen. Multiple collisions of counter-rotating waves have been discovered to be the primary mechanism in the CRDW stabilization process. There was a balance between gaining and losing energy for counter-rotating waves, culminating in a CRDW mode transition or CRDW extinguishment. The enhanced ignition intensity, equivalence ratio, and MFR produced the expected increase in CRDW intensity in the biogas-fuelled RDE. Enhancing these parameters aided in boosting the detonability of the biogas-air mixture. Quasi one-wave CRDW was observed from the start of ignition in all parametric cases, showing that the state of chaotic detonation instability was hardly occurred using biogas. To conclude, the current study discovered that the CRDW from the biogas-fuelled RDE has a more comprehensive operating stability range than the hydrogen-fuelled counterpart. Still, the rapid biogas detonation decay highlights the necessity for an enhanced mixing rate to preserve detonation continuity. The assessment of CRDW instabilities in the current study is pivotal for ensuring that these instabilities are effectively regulated and taken into account during the establishment of a RDE powered by biogas. The findings will also spearhead further research into parameters that could sustain CRDWs in the future working prototype of biogas-fuelled RDE.

ABSTRAK

Enjin ledakan berputar (RDE) digerakkan dengan biogas memberikan sumbangan kepada penciptaan enjin pembakaran yang dikuasakan oleh bahan bakar berasaskan tenaga boleh diperbaharui. Tetapi, potensi biogas RDE tidak pernah disiasat secara menyeluruh berdasarkan kritikal parameter operasi seperti intensiti pencucuhan, nisbah kesetaraan, dan kadar aliran jisim total (MFR). Jadi, tujuan utama kajian berangka ini adalah untuk meramal kestabilan perambatan gelombang ledakan berputar berterusan (CRDW) di RDE yang dibekalkan dengan hidrogen dan biogas berdasarkan impak parameter di atas. Untuk mewakili kestabilan CRDW, model berangka CRDW telah dibina. Satu model kimia satu langkah diubah suai telah dibina untuk peledakan biogas dan telah digabungkan dengan model berangka CRDW. Penilaian parametrik terhadap parameter ini telah dijalankan melalui model berangka CRDW yang telah disahkan bersama-sama model kimia satu langkah diubah suai untuk peledakan biogas. Ramalan tekanan CRDW telah berjaya disahkan dengan eksperimen dengan ralat kurang dari 10%. Model kimia satu langkah ini juga telah dibandingkan dengan eksperimen dan mekanisme terperinici, yang mana perbezaan masing-masing adalah 15.75% dan 8.29% terhadap halaju peledakan telah diperhatikan. Keputusannya, di persekitaran kurang bahan bakar dan tanpa pra-campuran dengan nilai pencucuhan sama, biogas RDE melebihi hidrogen RDE dari segi kestabilan peledakan yang mana ramalan masa untuk mencapai satu gelombang stabil di biogas RDE adalah 1327 mikrosaat lebih pendek dari hidrogen RDE. Namun, biogas RDE kurang dari segi keberlanjutan peledakan seperti yang diramalkan melalui kesinambungan gelombang. Selepas 0.0146 saat dari kemunculan satu gelombang stabil, RDW telah terpadam di biogas RDE tetapi hanya berlaku 1.52% pengurangan tekanan CRDW di hidrogen RDE. Asas penjelasan kepada perkara ini ialah biogas, yang mempunyai difusitiviti dan kereaktifan yang lebih rendah daripada hidrogen, mewujudkan ketidakseimbangan dalam gelombang putaran balas, dan menghasilkan peralihan mod CRDW yang lebih cepat daripada hidrogen. Perlanggaran berbilang gelombang putaran balas telah ditemui sebagai mekanisme utama dalam proses penstabilan CRDW. Terdapat keseimbangan antara memperoleh dan kehilangan tenaga untuk gelombang berputar balas, yang memuncak dalam peralihan mod CRDW atau pemadaman CRDW. Penggunaan intensiti penyalaan, nisbah kesetaraan dan MFR yang tinggi dijangka meningkatkan intensiti CRDW kerana peningkatan parameter ini akan menghasilkan keupayaan ledakan yang lebih tinggi untuk campuran biogas-udara. Kuasi satu gelombang CRDW berlaku dari awal pencucuhan di kesemua kes parametrik, menunjukkan ketidakstabilan ledakan sukar untuk dicapai melalui biogas. Kesimpulannya, CRDW dalam biogas RDE mempunyai julat kestabilan yang lebih luas daripada hidrogen RDE. Tetapi, pereputan ledakan biogas yang cepat menyerlahkan keperluan untuk meningkatkan kadar pencampuran untuk mengekalkan kesinambungan ledakan. Penilaian ketidakstabilan CRDW dalam kajian semasa adalah penting untuk memastikan ketidakstabilan ini dikawal dengan berkesan dan diambil kira semasa pembinaan biogas RDE. Penemuan ini juga akan menjadi batu loncatan untuk penelitian lebih lanjut parameter yang dapat memanjangkan keberlanjutan CRDW dalam biogas RDE.

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LIST OF ABBREVIATIONS

RDE	-	Rotating detonation engine
CRDW	-	Continuous rotating detonation wave
MFR	-	Total mass flow rate
SST	-	Shear stress transport
PDE	-	Pulse detonation engine
DT	-	Detonation tube
RANS	-	Reynolds-averaged Navier–Stokes
DDT	-	Deflagration to detonation transition
CJ	-	Chapman-Jouguet
ZND	-	Zeldovich-von Neumann-Döring
LHV	-	Lower heating value
LIH	-	Lavrentyev Institute of Hydrodynamics
TRL	-	Technology Readiness Level
HiREF	-	High Speed Reacting Flow Research Laboratory
UTM	-	Universiti Teknologi Malaysia
NASA	-	National Aeronautics and Space Administration
ROP	-	Rate of development
DAQ		Data acquisition
DNS	-	Direct Numerical Simulation
LES	-	Large Eddy Simulation
CFD	-	Computational fluid dynamics
3D	-	Three-dimensional
2D	-	Two-dimensional
NS	-	Navier–Stokes
RNG	-	Re-normalisation group
RSM	-	Reynolds stress equation model
CEA	-	Chemical equilibrium with applications
EDC	-	Eddy Dissipation Concept
AUSM	-	Advection Upstream Splitting Method
PT	-	Pressure transducer

PT1 - Pressure transducer 1
PT2 - Pressure transducer 2
CPU - Central processing unit
a.c. - Alternating current
d.c. - Direct current
RV - Reducing valve
MV - Magnetic valve
CV - Check valve
SP - Spark plug
M - Ignition modular
C - Ignition coil
PC - Personal computer
RT2 - Rectifier
D2 - Diode
C2 - Capacitor arrangement
RL2 - Relay
SWACER - Shock wave amplification by coherent energy release
ER0.6 - Equivalence ratio of 0.6
ER0.7 - Equivalence ratio of 0.7
ER0.8 - Equivalence ratio of 0.8
ER0.9 - Equivalence ratio of 0.9
ER1.0 - Equivalence ratio of 1.0
MF0.16 - Total mass flow rate of 0.16
MF0.26 - Total mass flow rate of 0.26
MF0.36 - Total mass flow rate of 0.36
MF0.46 - Total mass flow rate of 0.46
MF0.56 - Total mass flow rate of 0.56

LIST OF SYMBOLS

ϕ - Equivalence ratio

N_2 - Nitrogen

CH_4 - Methane

CO_2 - Carbon dioxide

OH - Hydroxyl radical

H - Hydrogen element

O - Oxygen element

T - Temperature

u - Velocity vector component in the x-direction

v - Velocity vector component in the y-direction

w - Velocity vector component in the z-direction

ρ - Density

P - Pressure

M - Mach number

$\dot{m}/A$ - Mass flux

Q - Heat addition

R - Specific gas constant

c_p - Specific heat capacity (constant pressure)

γ - Specific heat ratio

A - Area

λ - Reaction progress variable

h - Specific enthalpy

c - Speed of sound

E_a - Activation energy

Δ - Change in a quantity

$\emptyset$ - Universalization of any variable

$\sum \dot{Q}$ - Net rate of heat added to the control volume

$\sum \dot{W}$ - Net rate of work done on the control volume

$\dot{Q}_s\Delta V$ - Rate of heat added or removed by heat source on the control volume

μ - One of the proportionality constants related to viscosity

λ_v - One of the proportionality constants related to viscosity

R_{ij} - Reynold stresses

k - Turbulent kinetic energy

ε - Rate of dissipation of turbulent kinetic energy

ω - Specific rate of dissipation

J_i - Diffusion flux of species *i*

R_i - Net rate of production of species *i* by chemical reaction

S_i - Rate of creation by addition from the dispersed phase plus any user-defined sources

N_R - Reaction number

$M_{w,i}$ - Molecular weight of species *i*

$\hat{R}_{i,r}$ - Arrhenius molar rate of creation/destruction of species *i* in reaction *r*

N - Number of species involves in the reaction

$v''_{i,r}$ - Stoichiometric coefficient for product *i* in reaction *r*

$v'_{i,r}$ - Stoichiometric coefficient for reactant *i* in reaction *r*

$k_{f,r}$ - Forward rate constant of reaction *r*

$k_{b,r}$ - Backward rate constant of reaction *r*

$C_{j,r}$ - Molar concentration of species *j* in reaction *r*

$\eta'_{j,r}$ - One of the rate exponents of species *j* in reaction *r*

$\eta''_{j,r}$ - One of the rate exponents of species *j* in reaction *r*

t - Time

Y_i^* - Fine-scale species mass fraction after reacting over the time scale, τ^*.

ζ^* - Length fraction of the fine scales

C_ξ - Volume fraction constant

C_τ - Time scale constant

Δt_1 - Non-reacting mixing phase (filling stage)

Δt_2 - Non-reacting mixing phase (filling stage)

Δt_3 - Reacting flow phase (combustion period)

T_m - Flow rate temperature

P_i - Ignition pressure

T_i - Ignition temperature

V_i - Ignition velocity

P_{CJ} - CJ ignition pressure

T_{CJ} - CJ ignition temperature

V_{CJ} - CJ ignition velocity

t_o - Time interval exceeding the time scales of the slowest variations from the largest eddies

$\bar{u}$ - Mean velocity

G_k - Generation of k

G_ω - Generation of ω

Γ_k - Effective diffusivity of k

Γ_ω - Effective diffusivity of ω

Y_k - Dissipation of k

Y_ω - Dissipation of ω

k_r - Generic rate constant

A_r - Pre-exponential factor

n - Temperature exponent

x - Upstream annulus offset length

$\alpha 1$ - Upstream annulus divergence angle

A1 - Number of fuel inlets

A2 - Distance between fuel and oxidizer inlets

A3 - Fuel inlet diameter

A4 - Annulus width

A5 - Inner annulus radius

A6 - Outer annulus radius

A7 - RDE body length

CHAPTER 1

INTRODUCTION

1.1 Background

The rotating detonation engine (RDE) is an ingenious energy conversion system in such it promises remarkable reduction in fuel consumption and emissions [1]. Utilisation of detonation mode is the pinnacle feature of a RDE as it has the capability to liberate energy much quicker than deflagration combustion mode which take place in the conventional gas turbine system [2]. To further enlighten the understanding of RDE working operation, two major modes of combustion needs to be described properly. Detonation and deflagration are referred as the supersonic and the subsonic combustion processes respectively. The detonation mode triggered by the initiation of shock wave propagates through the flammable mixture with a supersonic speed. The characteristics of detonation including high thermal efficiency, rapid release of energy, and shockwave across the combustion region, and thus, makes it favourable in power and propulsion studies.

A RDE not only has all of the advantages of detonation, but also has the advantage of the compact and simple structure. With pressure gain attribute in detonation phenomenon, it can minimise the pressure that is required to compress the incoming air in the gas turbine system, thus, contribute to less compressor stages as compared to the conventional gas turbine systems. The current gas turbine systems utilise deflagration mode to burn the reactant mixture. The deflagration mode requires multi-stages compressors to elevate the pressure prior to being burned in a combustor. Therefore, the implementation of a RDE can simplify the engine structure, reduce the engine weight, and decrease the fuel consumption [2]. A RDE can provides nearly constant thrust using continuous rotating detonation waves (CRDWs) [2]. The concept of CRDW in a RDE makes it a better energy conversion system than the prior detonation-based energy conversion system; the pulse detonation engine (PDE) which used intermittent detonations [3-4].

The concept of a non-fossil fuel economy has now become the target of many regions around the world. In the spirit of developing a novel combustion engine powered by renewable-based fuels, the already novel RDE, when combined with the potential to operate with renewable-based fuels such as biogas and green hydrogen, will create a major contribution to the creation of a novel combustion engine powered by renewable-based fuels. With its high potential for incorporation into a gas turbine system by replacing the traditional deflagration combustion mode, the future of a RDE powered by renewable-based fuels is bright. As a result, the RDE system will bring an innovative revolution to existing power generation, aviation, and aerospace propulsion systems, as well as contribute to the reduction of global warming [5]. To accomplish this aim, the creation of a dependable and functional RDE system powered by renewable-based fuels such as biogas and green hydrogen is needed.

1.2 Problem Statement

In experiments to detect CRDWs in RDEs, pressure transducer and ion probe readings are commonly used [2]. Despite the vast amount of experimental data that can be taken from these sensors and exploited to discover different CRDW peculiarities [2], there is still a lack of information as there is a dearth of an overall picture of the CRDW process due to experimental setup constraints. Having said that, the point-based readings from the pressure transducer and the ion probe are insufficient to provide complete insights into CRDW dynamics. The constraints of experimental methodologies for displaying CRDW dynamics hampered in-depth understanding of CRDW phenomena, particularly CRDW stabilization and sustainability. When compared to experiments, numerical analysis can greatly improve and simplify CRDW visualisation. However, the lack of reliable numerical models that can improve understanding of CRDW stabilization will result in major instabilities not being properly identified during the CRDW stabilization stage, and the "indiscernible" difficulties not being appropriately addressed in order to construct a workable RDE, particularly one powered by biogas or hydrogen. Therefore, in order to construct a feasible RDE system, a credible numerical model that can improve understanding of CRDW stabilization and sustainability is required, which will eventually be employed for simulation-based design processes. A reliable numerical model can also be used to optimise RDE injection structures in order to improve mixing processes in the RDE annulus, which appears to be lacking in experimental studies that have leveraged the advantage of the RDE numerical model to improve mixing processes.

The chemistry model is one of the most critical factors to take into account when constructing a reliable numerical model that can accurately predict the CRDW dynamics in RDEs. The development of an appropriate chemistry model for biogas detonation is critical for predicting CRDW dynamics in a biogas-fuelled RDE. The validation feedback loop at varied constants in a chemistry is often executed until the simulation results agree well with the experimental data. While there is almost no experimental study on the use of biogas in RDEs, there are a few experimental publications, such as Wahid [6], Ghazali [7], and Elhawary [8], that have experimentally tested biogas detonation on detonation tube-based engines The fitting of a chemical model to simulate biogas detonation is critical because the comparatively low reactivity and diffusivity of biogas [9] could leads in diverse reacting flow dynamics in RDEs. If the chemistry model is not calibrated to represent biogas detonation, significant CRDW phenomena such as CRDW stabilization [10-11], unstable CRDWs [12], and detonation extinguishment [13-19] cannot be accurately captured in a biogas-fuelled RDE.

While there have been a number of detonation studies that have employed one-step and two-step Arrhenius chemistry models to account for both the accuracy and efficiency of detonation modelling [20-31], all of these studies addressed hydrogen detonation and hence used a hydrogen-air/oxygen chemistry model. Therefore, the published one-step chemical models have not been validated or tuned for biogas detonation modelling. As a result, there is some doubt about the credibility of the published one-step Arrhenius chemistry model to well predict the detonation behaviour in biogas-fuelled RDEs, as there is a high possibility that the published one-step models will produce ignition delay times that are a few orders of magnitude different than the ignition delay times from biogas detonation [32]. To appropriately model the CRDW from the biogas-powered RDE, the constant in the one-step Arrhenius chemistry model should be adjusted via the validation feedback loop to reflect the biogas detonation experimental data.

In terms of RDE systems, the construction of a fuel-lean non-premixed RDE is appealing in terms of safety and fuel consumption reduction. Nonetheless, in terms of CRDW dynamics, previous studies have found a number of serious concerns with the CRDW sustainability in a non-premixed RDE, the most notable of which being CRDW stability and longevity. Because hydrogen is the most commonly investigated fuel in the realm of RDE research, the majority of these issues were discovered in hydrogen-fuelled RDEs. Several research have already discovered the transient stabilization period for achieving a stable CRDW. Both Ma [10] and Liu [11] have scrutinized the events that lead to the formation of a stable CRDW. However, both of these references used premixed reactants. There are scenarios in non-premixed cases where it ends up producing unstable CRDWs [12] or even worse, the detonation extinguishment happened [13-18]. The phenomenon of detonation extinguishment in a non-premixed RDE is much more common in which a detonation failed to be created in the RDE annulus, ends up becoming a normal deflagration or no combustion at all. In a leaner equivalence ratio, the severity of CRDW instabilities was observed to be worsened [19]. All of these findings indicate that there is still a significant knowledge gap on the CRDW stabilization process in a fuel-lean non-premixed RDE, with one of the key reasons being the limits in experimental methodologies for visualising CRDWs, which inhibited in-depth understanding of CRDW dynamics. Characterization of instabilities during the CRDW stabilization process in a fuel-lean non-premixed RDE is critical to ensure that instabilities are adequately regulated and taken into consideration during the development of a fuel-lean non-premixed RDE, especially one powered by biogas or hydrogen.

The biogas-fuelled detonation engine, however, is not a new concept. In fact, studies have previously been conducted to evaluate biogas detonation with an emphasis on practical use of the detonation engine [6-8]. Nonetheless, all of these studies have concentrated on detonation tube-based applications, such as the PDE, which have a lower detonation frequency than a more novel detonation engine, such as the RDE. Hence, it is difficult to achieve a high detonation frequency in a PDE powered by low reactivity fuels such as pure biogas [6-8], making it unsuitable for practical usage. That being said, the CRDW, a quasi-continuous detonation with constant thrust in a RDE, could be the suitable combustion mechanism to allow the use of low reactivity fuels like biogas in detonation-based engines. However, hardly no study has been conducted on the use of biogas for RDEs. To investigate the potential of CRDWs in a biogas-fuelled RDE, a parametric assessment of critical operating parameters must be carried out. The equivalence ratio [2, 17, 19], mass flow rate [16, 24,] and ignition intensity [26, 76] are all significant operating parameters in RDE systems that have been examined previously. Despite this, there have been almost no studies that have investigated the effects of these parameters on CRDW stability in a biogas-fuelled RDE. As a result, the potential of a biogas-fuelled RDE has never been thoroughly investigated, leaving this type of engine with an unknown potential.

1.3 Research Questions

The research questions are:

(a) In comparison to experimental data, how accurate is the numerical model based on the Reynolds-averaged Navier–Stokes (RANS) equation and the one-step Arrhenius chemistry model in predicting the CRDW behaviour in RDEs?

(b) Is the above-mentioned numerical model capable of reasonably predicting the transitory detonation stabilization phase in RDEs?

(c) Is the modified one-step chemistry model capable of reasonably predicting the occurrence of biogas detonation?

(d) Does the biogas-fuelled RDE used in the present study have a transitory detonation stabilization phase? If so, how does the transitory detonation stabilization phase from the biogas-fuelled RDE vary from the hydrogen-fuelled RDE?

(e) What is the expected intensity and stability of CRDWs in fuel-lean non-premixed biogas- and hydrogen-fuelled RDEs?

(f) What is the expected intensity and stability of CRDWs in the biogas-fuelled RDE at different ignition intensities, equivalence ratios, and mass flow rates?

1.4 Research Objectives

The research objectives are:

(a) To establish the validated numerical model of CRDW based on the detonation experimental data.

(b) To establish a comprehensive comparative assessment of CRDW behaviour from fuel-lean non-premixed biogas- and hydrogen-fuelled RDEs.

(c) To predict the impact of ignition intensity, equivalence ratio, and mass flow rate towards the CRDW stability in the biogas-fuelled RDE.

1.5 Scopes of Research

The scopes of the present research are as follows:

(a) The CRDW simulation in the hydrogen-fuelled RDE is limited to a single case as the baseline. The subsequent parametric studies are only for the biogas-fuelled RDE.

(b) For objective (a), both experimental and numerical methods are used to establish the validated numerical model of CRDW.

(c) For objectives (b) and (c), numerical methods are employed using the established validated numerical model in objective (a).

(d) To capture the mixing process and CRDW behaviour, both non-reacting and reacting flows are transiently modelled.

(e) The only geometry covered in the current analysis is the RDE body, which plays a significant role in the flow dynamics behaviour within the RDE system.

(f) The current research focuses solely on the intensity and stability of CRDW in the biogas-fuelled RDE in terms of the predicted pressure front, as this is the most common parameter examined in experimental studies via pressure transducer readings. To back up the pressure front findings, the predicted heat of reaction rate is also analysed.

(g) The predicted CRDW stability in the biogas-fuelled RDE is investigated via the decay of CRDW pressure and heat of reaction over time, with simulation time limited to the 12th cycle of CRDW propagation to balance simulation accuracy and efficiency.

(h) The parameters studied in the biogas-fuelled RDE parametric studies are only the ignition intensity, equivalence ratio, and total mass flow rate.

(i) Since it is the most typical biogas composition in the literature, this analysis only covers biogas with a composition of 65% methane (CH_4) and 35% carbon dioxide (CO_2). The impact of varying biogas composition on the CRDW stability is left for future research.

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