# SIMULATION MODELS TO OPTIMISE HYDROGEN FUELLED ENGINE PERFORMANCE

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Thesis submitted in fulfilment of the requirements for the award of the degree of Doctor of Philosophy in Mechanical Engineering (Automotive)

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2011

## SUPERVISORS' DECLARATION

We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Doctor of Philosophy in Mechanical Engineering (Automotive).

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I hereby declare that the work in this thesis is my own except for quotations and summaries, which have been duly acknowledged. The thesis has not been accepted for any degree and is not concurrently submitted for award of other degree.

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## List of Symbols

| Symbol | Description | Unit |
|---|---|---|
| $a$ | Crank radius | m |
| $A$ | Combustion chamber surface area | m$^2$ |
| $a_{1-}a_7$ | The coefficients of NASA and Chemkin Polynomials | - |
| $A_1$ and $A_1$ | Constants in Karim's correlation for combustion duration | - |
| $A_3$ and $A_4$ | Constants in Karim's correlation for flame development angle | - |
| $a_{An}$ | Constant in Annand's correlation | - |
| $A_C$ | Valve curtain reference area | m$^2$ |
| $A_{ch}$ | Cylinder head surface area | m$^2$ |
| $A_{cf}$ | The constant part of the *FMEP* in Chen-Flynn friction model | bar |
| $A_E$ | Valve throat effective area | m$^2$ |
| $AFR$ | Air/fuel ratio | - |
| $A_i$, $B_i$, $C_i$, $D_i$, $E_i$ | Coefficients for calculating the chemical equilibrium constant | - |
| $AFR_s$ | Stoichiometric air/fuel ratio | - |
| $A_n$ | The total injector nozzle hole area | m$^2$ |
| $A_{pc}$ | Piston crown surface area | m$^2$ |
| $A_R$ | Valve throat reference area | m$^2$ |
| $a_s$ | Molar hydrogen air/fuel ratio | - |
| $a_W$ | Adjustable factor in Wiebe's function | - |
| $B$ | Cylinder bore | m |
| $B_{cf}$ | Peak cylinder pressure dependent factor in Chen-Flynn friction model | - |
| *BMEP* | Brake mean effective pressure | kPa |
| $BSFC$ | Brake specific fuel consumption | g/kW-h |
| $C'$ | Calibration factor in Karim's correlation for combustion | - |
| $C''$ | Calibration factor in Karim's correlation for flame development angle | - |

| **Symbol** | **Description** | **Unit** |
|---|---|---|
| $C_1$ and $C_2$ | Constants in Woschni's correlation | - |
| $C_2^*$ | Corrected coefficient for the constant $C_2$ in Woschni's correlation proposed by (Kolesa, 1987) and Schwarz (1993) | - |
| $C_c$ | Calibration parameter in the Bargende's correlation | - |
| $C_{cf}$ | $\bar{S}_p$ dependent term in Chen-Flynn friction model | bar/(m/sec) |
| $C_D$ | Discharge coefficient | - |
| $C_{D,i}$ | Injector discharge coefficient | - |
| $C_{ff}$ | Coefficient for the cam flat follower in friction model | kPa-mm |
| $C_{oh}$ | Coefficient for oscillating hydrodynamic in friction model | (KPa-mm-min/rev)$^{1/2}$ |
| $C_{om}$ | Coefficient for oscillating mixed friction in friction model | kPa |
| $C_p$ | Specific heat at constant pressure | |
| $C_{rf}$ | Coefficient for the cam roller follower in friction model | (kPa-mm-min/rev) |
| $C_V$ | Specific heat at constant pressure | kJ/kg-K |
| $D$ | Diameter of the sphere which has the same volume as the cylinder in Bargende's correlation | m |
| $D_b$ | Bearing diameter | m |
| $D_m$ | Mean valve seat diameter | m |
| $D_p$ | Port diameter | m |
| $D_s$ | Valve stem diameter | m |
| $D_v$ | Valve diameter | m |
| $e$ | Total specific energy | kJ/kg |
| $E_{sys}$ | Total energy of the thermodynamic system | kJ |
| $e_t$ | Tolerance | - |
| $FAR$ | Fuel/air ratio | - |
| $FAR_s$ | Stoichiometric fuel/air ratio | - |
| $FMEP$ | Friction mean effective pressure | kPa |
| $G$ | Gibbs free energy | kJ |
| $h$ | Specific enthalpy | kJ/kg |
| $H$ | Enthalpy | kJ |

| **Symbol** | **Description** | **Unit** |
|---|---|---|
| $h_c$ | Heat transfer coefficient | W/m$^2$-K |
| $h_{clr}$ | Clearance height | m |
| $h_i$ | Specific enthalpy of in- flowing gases | kJ/kg |
| $h_o$ | Specific enthalpy of out-flowing gases | kJ/kg |
| $H_p$ | Products enthalpy | kJ |
| $H_r$ | Reactants enthalpy | kJ |
| $IMEP$ | Indicated mean effective pressure | kPa |
| $ISFC$ | Indicated specific fuel consumption | g/kW-h |
| $k$ | The turbulent kinetic energy | m$^2$/s$^2$ |
| $K$ | Constant in friction model | - |
| $K_c$ | Thermal conductivity | W/m-K |
| $K_p$ | Equilibrium constant | - |
| $l$ | Connecting rod length | m |
| $L$ | Piston stroke | m |
| $L_b$ | Bearing length | m |
| $L_c$ | Length scale in Nusselt number | m |
| $LHV$ | Lower heating value | MJ/kg |
| $l_I$ | Length scale in the $k-\varepsilon$ turbulence model | m |
| $l_v$ | Valve lift | m |
| $m$ | Mass | kg |
| $M$ | Molecular weight | kg/kmol |
| $\dot{m}$ | Mass flow rate | kg/s |
| $\dot{m}_a$ | Air mass flow rate | kg/s |
| $\dot{m}_{act}$ | Actual mass flow rate | kg/s |
| $MEP$ | Mean effective pressure | kPa |
| $m_f$ | Fuel mass | kg |
| $\dot{m}_f$ | Fuel mass flow rate | kg/s |
| $MFB$ | Mass fraction burned | - |
| $m_i$ | Mass flow entering the cylinder | kg/s |

| **Symbol** | **Description** | **Unit** |
|---|---|---|
| $m_o$ | Mass flow out of the cylinder | kg/s |
| $m_{rg}$ | Mass of the residual gas | m |
| $m_{sys}$ | Net mass flow for the cylinder | kg/s |
| $m_{tot}$ | Total mass in the cylinder | m |
| $\dot{m}_{theo}$ | Theoretical mass flow rate | kg/s |
| $m_W$ | Wiebe form parameter | - |
| $n$ | Polytropic index | - |
| $N$ | Engine speed | rpm |
| $n_b$ | Number of bearing | - |
| $n_c$ | Number of cylinders | - |
| $n_i$ | Number of moles of the chemical constituents | mole |
| $N_m$ | Total number of moles | mole |
| $N_p$ | Engine maximum speed | rpm |
| $Nu$ | Nusselt number | - |
| $n_v$ | Number of valves | - |
| $p$ | Pressure | kPa |
| $p_0$ | Total mixture pressure | kPa |
| $p_a$ | Pressure after valve restriction in the direction of flow | kPa |
| $p_{atm}$ | Atmospheric pressure | kPa |
| $p_b$ | Pressure before valve restriction in the direction of flow | kPa |
| $P_b$ | Brake power | kW |
| $p_{comb}$ | Pressure at the beginning of the combustion process | kPa |
| $p_e$ | Exhaust pressure | kPa |
| $P_f$ | Friction power | kW |
| $p_i$ | Constituent partial pressure | kPa |
| $P_i$ | Indicated power | kW |
| $p_{in,man}$ | Intake manifold pressure | kPa |
| $p_m$ | Motored cylinder pressure | kPa |
| $p_{max}$ | Maximum cylinder pressure | kPa |

| Symbol | Description | Unit |
|---|---|---|
| $p_r$ | Reference pressure for Woschni's correlation | kPa |
| $Pr$ | Prandtl number | - |
| $Q_{cf}$ | $\bar{S}_p^2$ dependent term in Chen-Flynn friction model | bar/(m/s$^2$) |
| $Q_{conv,total}$ | Fraction of the total energy converted by combustion process | - |
| $Q_{f,total}$ | Total energy released from combustion | kJ |
| $Q_w$ | Heat transfer | kJ |
| $R$ | Gas constant | kJ/kg-K |
| $r_e$ | Exhaust valve diameter/bore ratio | - |
| $Re$ | Reynolds number | - |
| $r_i$ | Intake valve diameter/bore ratio | - |
| $\tilde{R}$ | Universal gas constant | J/kmole-K |
| $s$ | Specific entropy | kJ/kg-K |
| $S$ | Entropy | kJ/kg |
| $s^o$ | Specific entropy when the partial pressure of the constituent equals the mixture pressure. | kJ/kg-K |
| $S_p$ | Instantaneous piston speed | m/s |
| $\bar{S}_p$ | Mean piston speed | m/s |
| $S_{re}$ | Summation of squares of residuals in the NLSR | - |
| $t$ | Time | s |
| $T$ | Temperature | K |
| $T_{gas}$ | Cylinder gases temperature | K |
| $T_0$ | Reference point temperature | K |
| $T_A$ | Ambient temperature | K |
| $T_{ad}$ | Adiabatic flame temperature | K |
| $T_b$ | Temperature before valve restriction in the direction of flow | K |
| $T_{bu}$ | The temperatures of the burned zone | K |
| $T_e$ | Exhaust temperature | K |
| $T_i$ | Intake charge temperature | K |
| $T_m$ | In-cylinder average temperature, used in Bargende's correlation | K |

| **Symbol** | **Description** | **Unit** |
|---|---|---|
| $T_r$ | Reference temperature for Woschni's correlation | K |
| $T_{sp}$ | Temperature at the spark discharge time | K |
| $T_{ub}$ | Temperatures of the unburned zone | K |
| $T_w$ | Cylinder wall temperature | K |
| $u$ | Specific internal energy | kJ/kg |
| $U$ | Internal energy | kJ |
| $v$ | Characteristic velocity in Reynolds number | m/s |
| $V$ | Volume | $m^3$ |
| $V_c$ | Clearance volume | $m^3$ |
| $V_{comb}$ | Volume at the beginning of the combustion process | $m^3$ |
| $V_d$ | Cylinder displacement volume | $m^3$ |
| $v_f$ | Velocity of hydrogen through nozzle | m/s |
| $V_r$ | Reference volume for Woschni's correlation | $m^3$ |
| $V_{sp}$ | Volume at the time of spark discharge | $m^3$ |
| $V_{spc}$ | Specific volume | $m^3$/kg |
| $w$ | Average cylinder gas velocity | m/s |
| $W$ | Work | kJ |
| $W_b$ | Brake work per cycle | kJ |
| $W_i$ | Indicated work per cycle | kJ |
| $W_{p,max}$ | Maximum injector pulse width | deg |
| $w_s$ | Valve seat width | m |
| $x$ | Mass fraction of the constituents | - |
| $x_{rg}$ | Residual gas mass fraction | - |
| $y$ | Mole fraction of the constituents | - |
| $y_{rg}$ | Residual gas mole fraction | - |
| $z$ | Distance between the crank axis and the piston pin axis | m |

## Greek Symbols

| Symbol | Description | Unit |
|---|---|---|
| $\Delta\theta_b$ | Rapid burn angle | deg |
| $\Delta\theta_d$ | Flame development angle | deg |
| $\Delta p_n$ | Pressure drop across the injector nozzle | kPa |
| $\eta_C$ | Combustion efficiency | - |
| $\eta_{ch}$ | Charge efficiency | - |
| $\eta_m$ | Mechanical efficiency | - |
| $\eta_{thb}$ | Brake thermal efficiency | - |
| $\eta_{thi}$ | Indicated thermal efficiency | - |
| $\eta_{v,p}$ | Volumetric efficiency calculated at the highest speed and WOT operation condition | - |
| $\eta_v$ | Volumetric efficiency | - |
| $\theta_{EOC}$ | Crankshaft position at combustion End | deg |
| $\theta_{SOC}$ | Crankshaft position at combustion start | deg |
| $\theta_{sp}$ | Crankshaft position at spark timing | deg |
| $\mu_0$ | Reference viscosity | cSt |
| $\rho_{a,i}$ | Inlet air density | $kg/m^3$ |
| $\rho_f$ | Fuel density | $kg/m^3$ |
| $\rho_v$ | Density used to calculate the volumetric efficiency $\eta_{v,p}$ | $kg/m^3$ |
| $\tau_w$ | Wall shear stress | $N/m^2$ |
| $\phi_l$ | Lean operation limit for fuel/air equivalence ratio | - |
| $\phi_{min}$ | Fuel/air equivalence ratio for minimum combustion duration | - |
| $\phi_r$ | Rich operation limit for fuel/air equivalence ratio | - |
| ~ | Superscript denotes that the property is calculated on molar basis | - |
| $\Delta$ | Combustion term in Bargende's correlation | - |
| $\Delta\tilde{h}_f^0$ | Standard enthalpy of formation | MJ/kmole |

| Symbol | Description | Unit |
|---|---|---|
| $\Delta G^0$ | Standard state Gibbs function change | kJ |
| $\Delta\theta_{CD,min}$ | Minimum combustion duration | deg |
| $\Delta\theta_{CD}$ | Combustion duration | deg |
| $\Delta\theta_{d,min}$ | Minimum flame development angle | deg |
| $\Pi$ | Pressure ratio over the valve restriction | - |
| $\Psi$ | Valve flow function | - |
| $\beta$ | Valve seat angle | rad |
| $\gamma$ | Specific heat ratio | - |
| $\varepsilon$ | Turbulence energy dissipation rate | $m^2/s^3$ |
| $\theta$ | Crankshaft angle | deg |
| $\lambda$ | Air/fuel relative ratio | - |
| $\mu$ | Dynamic viscosity | Pa.s |
| $\rho$ | Density | $kg/m^3$ |
| $\omega$ | Angular velocity | rad/s |
| $\epsilon$ | Compression ratio | - |
| $\phi$ | Fuel/air equivalence ratio | - |

# LIST OF ABBREVIATIONS

| | |
|---|---|
| 1D | One dimensional |
| AFR | Air fuel ratio |
| BPI | Borderline for pre-ignition |
| BSFC | Brake specific fuel consumption |
| CAE | Computer added engineering |
| CFR | Cooperative Fuel Research |
| CR | Common rail |
| CRIS | Common Rail Injection System |
| DI | Direct Injection |
| $DIH_2ICE$ | Direct Injection Hydrogen Fuelled Internal Combustion engine |
| DOCS | Double Overhead Camshaft |
| ECU | Electronic control unit |
| EGR | Exhaust gas recirculation |
| EIA | Energy Information Administration |
| EOC | End Of Combustion |
| EU 5 | European emission standards until 2008/2009 |
| FAR | Fuel air ratio |
| FMEFcs | Crankshaft friction mean effective pressure |
| FMEFgasL | Friction mean effective pressure in the reciprocating components due to gas pressure loading |
| FMEFpl | Pumping losses friction mean effective pressure |
| FMEFrecip | Friction mean effective pressure in the reciprocating components without gas pressure loading |
| FMEP | Friction mean effective pressure |
| FMEP | Brake mean effective pressure |
| FMEPaux | Auxiliary components friction mean effective pressure |
| FMEPvt | Valvetrain friction mean effective pressure |
| $H_2ICE$ | Hydrogen fuelled internal combustion engine |
| $H_2R$ | Hydrogen record car |

| | |
|---|---|
| HTFL | Heat transfer first law approach |
| IC | Internal Combustion |
| ICE | Internal Combustion Engine |
| IEA | International Energy Agency |
| IMEP | Indicated mean effective pressure |
| IPHE | International Partnership for the Hydrogen Economy |
| ISFC | Indicated specific fuel consumption |
| IT | Injection Timing |
| LHV | Lower Heating Value |
| LLSR | Linear Least Squares Regression |
| MAP | Manifold absolute pressure |
| MBT | Minimum advance for best torque |
| MEP | Mean effective pressure |
| MOSTI | Ministry of Science, Technology and Innovation Malaysia |
| NBS | National Bureau of Standards |
| NLSR | Nonlinear Least Squares Regression |
| $NO_x$ | Nitric oxides emissions |
| OH | Hydroxide |
| PI | Port Injection |
| PIFL | Polytropic index first law approach |
| $PIH_2ICE$ | Port Injection Hydrogen Fuelled Internal Combustion engine |
| PLIF | Planar Laser Induced Fluorescence |
| R&D | Research and Development |
| RM | Ringgit Malaysia |
| SFC | Specific fuel consumption |
| SOC | Start of combustion |
| SOCS | Single overhead camshaft |
| ST | Spark timing |
| TDC | Top dead centre |
| TLEV | Transitional low emission vehicles |

| | |
|---|---|
| USD | United States Dollar |
| UV | Ultraviolet |
| V | V engine or Vee engine. |
| VCS | Villars-Cruise-Smith equilibrium code |
| WOT | Wide open throttle |

# ABSTRACT

Hydrogen is a strong candidate as an alternative fuel and energy carrier which could address answers to environmental pollution, emissions and geo-political tensions. This thesis aims to develop modeling codes for rapid simulation and optimisation for hydrogen fuelled engines ($H_2$ICE). A composition and property model is developed for calculating the composition and thermodynamic properties of the multi-components gases in the $H_2$ICE. The framework of this model encapsulates all possible situations from gases that are modelled on a molecular level to gases that are modelled as fresh air with some residuals. A one-dimensional model for a port injection $H_2$ICE is also developed. This model uses a single-zone approach and simulates the different physical phenomena in the intake, compression, combustion and expansion processes. Previous models for heat transfer and heat release are introduced for hydrogen applications after proposing suitable modifications and calibrating factors. In addition, computational models are developed to investigate and optimise injection characteristics in direct injection $H_2$ICEs as well as common rail port injection fuelling system. Following this, a one dimensional model is developed for an engine with dual pure fuels and blended fuels. The considered fuels are hydrogen, gasoline, methane, gasoline-hydrogen blends and methane-hydrogen blends. These models have been calibrated and validated against experimental works and the findings of previous studies. The results have showed the accuracy of the composition and property code and that it is a very useful tool for $H_2$ICE simulations. Less than 0.3% deviation has been noticed for the entire considered range of temperature and equivalence ratio ($\phi$). In addition, the port injection code has highlighted that spark timing as a very important contributor among the different parameters and how an optimisation for these contributors can enhance the performance. A calibration factor of 2.183 has been proved to give accurate results for the new heat transfer correlation. Besides, the deviation in the results of the heat release model was 2.3% in the worst case. From the injection models, it was shown that optimizing the injection parameters, in particular injection timing, are very crucial factors for engine performance and proper operation for the feeding system. The performance of $H_2$ICE in comparison with engines use other fuels was investigated using the dual fuel model. Hydrogen fuel showed its superiority in the lean conditions ($\phi$ < 0.4). Furthermore, the penalty and benefits from hydrogen enrichment were clarified. It was shown that adding small controllable mass factions of hydrogen (< 10%) to gasoline enhances the burning velocity and combustion process in the low speed range. However, a small reduction in the output power (< 6%) was documented. Adding hydrogen to methane showed greater advantages due to the extremely low burning velocity of methane. It can be recognized that the developed simulation codes are powerful tools for the $H_2$ICE community. With these models, experiments can be supplemented and supported by fast calculations.

# ABSTRAK

Hidrogen ialah calon terbaik sebagai bahan bakar alternatif dan pembawa tenaga yang dapat menyelesaikan permasalahan pencemaran alam sekitar, emisi dan ketegangan geo-politik. Thesis ini menumpukan kepada pembangunan model untuk simulasi pantas dan optimisasi enjin dengan bahan bakar hidrogen. Sebuah model komposisi dan ciri telah dibangunkan untuk menyelesaikan pengiraan komposisi dan ciri termodinamik bagi pelbagai komposisi gas di dalam enjin hydrogen. Rangka kerja model ini meliputi pelbagai kemungkinan keadaan gas yang dimodelkan pada tahap molekul sehingga kepada pemodelan gas yang mengandungi udara segar dan sedikit gas baki. Model satu dimensi untuk enjin hidrogen bersuntikan pancarongga juga telah dibangunkan. Pendekatan satu dimensi telah digunakan untuk mensimulasi beberapa fenomena fizikal yang berbeza semasa proses masukan, mampatan, pembakaran dan pengembangan.
Beberapa model terdahulu bagi pembebasan dan pemindahan haba telah digunakan untuk aplikasi hidrogen setelah mengambilkira beberapa pengubahsuaian dan faktor kalibrasi. Tambahan lagi, model berkomputer juga telah dibangunkan untuk menyiasat dan mengoptimumkan ciri suntikan bagi suntikan terus dan suntikan pancarongga enjin pembakaran dalam dengan bahan bakar hidrogen. Seterusnya, model satu dimensi juga telah dibangunkan bagi enjin yang menggunakan bahan bakar duaan dan bahan bakar campuran. Bahan api yang dikaji adalah hidrogen, petrol, metana, campuran petrol-hidrogen, dan juga campuran metana-hidrogen. Model ini telah dikalibrasi dan disahkan dengan menggunakan data eksperimen dan penemuan daripada kajian yang terdahulu. Keputusan menunjukkan ketepatan hasil pengiraan program komposisi dan ciri yang terdahulu dan membuktikan kebergunaannya untuk simulasi enjin pembakaran dalam hydrogen. Jurang pengiraan adalah kurang daripada 0.5% bagi kesemua julat suhu dan nisbah kesetaraan yang diambilkira. Sebagai tambahan, bagi suntikan pancarongga, keputusan telah menunjukkan bahawa pemasaan pencucuhan adalah factor terpenting yang menyumbang kepada penambahbaikan prestasi enjin berbanding beberapa parameter lain dan bagaimana parameter ini dioptimumkan. Faktor kalibrasi sebanyak 2.183 membuktikan kemampuan korelasi pemindahan haba mampu memberikan hasil pengiraan yang tepat. Selain daripada itu, jurang perbandingan terbesar sebanyak 2.3% telah dikenalpasti bagi model pelepasan haba. Daripada model suntikan, telah ditunjukkan bahawa proses optimisasi parameter suntikan, khususnya pemasaan suntikan sangat penting bagi prestasi enjin dan pengoperasian system campuran enjin yang lebih baik. Prestasi enjin hidrogen telah dibandingkan dengan enjin yang menggunakan bahan bakar berbeza dengan menggunakan model bahan bakar duaan. Enjin hidrogen telah menunjukkan kelebihannya yang ketara untuk operasi campuran rendah dimana nilai nisbah kesetaraannya adalah kurang dari 0.4. Sebagai tambahan, kelemahan dan kelebihan daripada pengayaan hidrogen telah berjaya dinyatakan secara jelas. Terbukti bahawa penambahan sejumlah amaun pecahan jisim hydrogen (kurang dari 10%) kepada petrol mampu meningkatkan prestasi halaju nyalaan dan proses pembakaran semasa julat halaju enjin yang rendah. Walau bagaimanapun, sedikit pengurangan daripada keluaran enjin (kurang dari 6%) telah dikenalpsti. Penambahan hidrogen kepada metana telah memberikan penambahbaikan yang lebih ketara akibat daripada halaju nyalaan asli metana yang sangat rendah. Secara umumnya, dapat dinyatakan bahawa model yang telah dibangunkan adalah alat bantu yang sangat berguna untuk komuniti kajian enjin pembakaran dalam hydrogen. Dengan menggunakan model ini, eksperimentasi dapat diperbaiki dan dibantu dengan suatu kaedah pengiraan yang pantas.

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