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MODELING THE COMBUSTION OF (M)ETHANOL IN SPARK-IGNITION ENGINES

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ABSTRACT –

Research and /or Engineering Questions/Objective: The use of light alcohols in spark-ignition engines is an interesting option to secure domestic energy supply and decarbonize transport. The impact of these fuels on engine control strategies can be explored at low cost using engine cycle simulations. Existing models, however, insufficiently account for the specific effects of alcohols on engine operation. The goal of the current work is thus to develop an engine cycle code that can accurately predict performance, efficiency, pollutant emission and knock onset in state-of-the-art neat alcohol engines.

Methodology – Quasi-dimensional engine modeling is put forward as a useful tool for cheap and fast optimization of engines. This model class derives the mass burning rate of fuel from turbulent combustion models. Previous work by the authors focused on obtaining reliable data for the laminar burning velocity of methanol and ethanol. This is a fundamental building block of any turbulent combustion model and groups the chemical effects of pressure, temperature, equivalence ratio and residual gas on combustion. Now, this data is implemented in an engine code and used to reproduce the experimental cylinder pressure traces obtained on three different flex-fuel engines. Additionally, these traces are used to compare various turbulent combustion models.

Results – Comparison of experimental and simulated cylinder pressure traces confirmed the predictive power of the developed engine cycle model. A wide variety of engine operating points on both methanol and ethanol were accurately reproduced thanks to the new laminar burning velocity data. Turbulent combustion models accounting for thermo-diffusive properties were shown to hold a slight edge over simpler formulations.

Limitations of this study – An important limitation of the current study is the absence of accurate estimations for the in-cylinder bulk flow and turbulence. Also, the current model is only validated for port-fuel injected engines. Further work will focus on the effects of direct injection and look at pollutant formation.

What does the paper offer that is new in the field in comparison to other works of the author – Compared to previous work the effects of in-cylinder pressure, temperature and mixture composition on the combustion are more accurately predicted thanks to the inclusion of new and widely validated laminar burning velocity data. In contrast to other studies, the current experimental database also includes measurements for a wide range of equivalence ratios and elevated amounts of exhaust gas recirculation.

Conclusion – The current work focused on adapting the various submodels of quasi-dimensional engine codes to the properties of light alcohols. The developed simulation tools can be used with confidence to optimize current and future engines running on neat methanol and ethanol.

TECHNICAL PAPER –

INTRODUCTION

Light Alcohols as SI Engine Fuels

Sustainable light alcohols such as methanol and ethanol are interesting alternative fuels for spark-ignition (SI) engines. They offer the prospect of CO_2 neutral transport and increased energy security, while ameliorating engine performance and efficiency compared to fossil fuels thanks to a number of interesting properties [1, 2]. The most significant interesting properties of light alcohols include:

- High heat of vaporization, which causes considerable charge cooling as the injected fuel evaporates.
- Elevated knock resistance, which allows applying higher compression ratios (CR), optimal spark timing and aggressive downsizing.

- High flame speeds, enabling qualitative load control using mixture richness or varying amounts of exhaust gas recirculation (EGR) [3].

The potential of neat light alcohol fuels (methanol and ethanol) has been demonstrated experimentally in both dedicated and flex-fuel alcohol engines [3]. Today, however, costly experimental tests are increasingly replaced by cheap system simulations of the engine. With current trends like alternative fuels, downsizing, EGR, multiple spark plugs per cylinder, etc. it is indeed no longer possible for an R&D engineer to intuitively grasp how these factors will affect the engine operation. The employed engine models are obviously required to reproduce any fuel specific effects on the combustion process.

Quasi-dimensional (QD) engine simulation codes are well suited to evaluate existing engines, perform parameter studies and predict optimum engine settings without resorting to complex multidimensional models [4]. The governing equations for such models are based on conservation of mass and energy. A two-zone formulation separates the burned from the unburned gases by an infinitely thin, spherically propagating flame front. At Ghent University, a QD code for the power cycle of hydrogen fueled engines has been developed and validated during earlier work (GUEST: Ghent University Engine Simulation Tool) [5]. The current work aims to extend this code to light alcohol fuels (i.e. methanol and ethanol) and to add models predicting the gas dynamics in engines running on these fuels.

SIMULATION PROGRAM

Framework and assumptions

The focus of this paper is the validation of turbulent combustion models for engine operation on neat methanol and ethanol. Also, the in-house GUEST code was coupled to a commercial gas dynamics simulation tool, to enable simulation of the entire engine cycle (GT-Power [6]).
The current two-zone QD power cycle model was derived using several standard assumptions, discussed in [5, 4]. The equations for the rate of change of the cylinder pressure $dp=d\theta$, burned and unburned temperatures, $dT_b=d\theta$ and $dT_u=d\theta$, are derived from conservation of energy. Additionally, a number of models and assumptions are necessary to close these equations. These are discussed in earlier publications [7].

Turbulent combustion model

A turbulent entrainment velocity u_{te} is needed for closure of the equations. A number of u_{te} models were selected through comparison against measurements of the turbulent burning velocity of methanol- and ethanol-air obtained during spherical explosions in a constant volume bomb [8, 9].
The models were implemented as summarized below. A full description of the different models can be found in the original references or in [8].

- Damköhler [10]:
  $u_t = C_2u' + u_n$ (1)
- Gülder [11]:
  $u_t = 0.6C_2u'^{0.5}u_n^{0.5}Re_t^{0.25} + u_n$ (2)
- Bradley KaLe [12]:
  $u_t = 0.88C_2u'(KaLe)^{-0.3} + u_n$ (3)
- Zimont [13, 14]:
  $u_t = C_2u'Da^{1/4} + u_n$ (4)
- Dinkelacker [15]:
  $u_t = u_n +(0.46C_2u_n/Le)Re_t^{0.25}(u'/u_n)^{0.3}(p/p_0)^{0.2}$ (5)

Richard et al. [16] have recently reduced their 3D Coherent Flame Model (CFM) to a formulation that is compatible with QD engine modeling. The model formulation can be found in [16].

C_2 is a calibration constant, u_n is the stretched laminar burning velocity, Ka is the Karlovitz stretch factor [12], Le is the Lewis number and Da is the Damköhler number which is calculated using a laminar flame thickness based on the kinematic viscosity ($\delta_l = \nu_u/u_l$). Alternatively, the flame thickness can be more precisely calculated using the δ_l correlations developed by the current authors [7, 8]. The best results were obtained without the use of a stretch model, i.e. $u_n = u_l$.

Laminar burning velocity correlation

Turbulent burning velocity models need (stretched) laminar burning velocity data of the air/fuel/residuals mixture at the instantaneous pressure and temperature. As of today, there are insufficient data on stretch-free

burning velocities at engine conditions, for any fuel. Stretch and instabilities hamper the experimental determination of stretch-free data at higher (engine-like) pressures [17].
The current authors have worked on the laminar burning velocity of methanol and ethanol mixtures, compiling data from the literature [18] and looking at numerical [18] as well as experimental [1, 19, 20] means to determine a suitable laminar burning velocity correlation. Laminar burning velocity correlations for methanol and ethanol have been determined based on chemical kinetics calculations [18]. These correlations have been extensively validated against measurements obtained on two different fundamental combustion research setups [1, 19, 20]. Figure 1 shows that, compared to the older correlations of Metghalchi & Keck and Gülder, the methanol u_l correlation developed by the current authors places the peak laminar burning velocity at a richer equivalence ratio and predicts a less steep decrease in u_l for rich mixtures. The residual gas correction term of Rhodes and Keck, developed for indolene/air/diluents mixtures, predicts a steeper drop in burning velocity in terms of diluents ratio than the other correlations. Similar observations can be made for the u_l correlations of ethanol (not shown here).

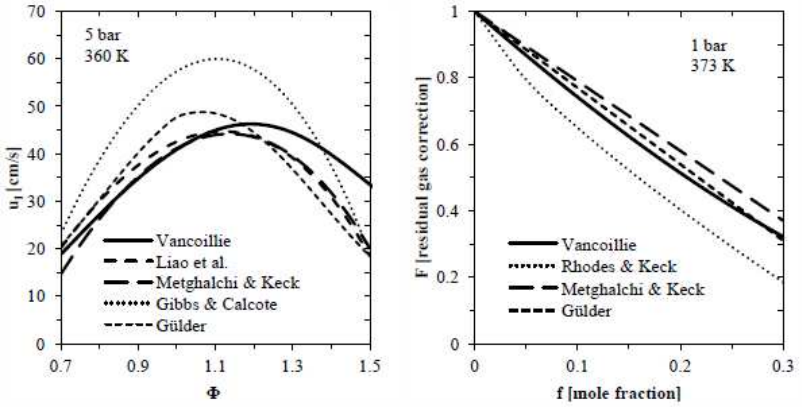

Figure 1. Comparison of predicted ul as a function of ϕ (left) and residual gas correction terms (right).
'Vancoillie' refers to the correlation developed in [18]

MODEL VALIDATION

Engine measurements

To validate the combustion and knock models' predictive capabilities, a series of measurements were done on a single cylinder Audi research engine. The engine and the employed measurement equipment have been discussed elsewhere [8, 21]. The main characteristics of the engine are summarized in Table 1.

Engine type	Audi
Cylinders	1
Valves	2
Valvetrain	Overhead cam
Bore	77,5 mm
Stroke	86,4 mm
Displacement	407,3 cc
CR	13,13 : 1
Injection	PFI
Induction	Atmospheric
ECU	MoTeC M4Pro

Table 1. Engine Specifications

The measurements comprise variable fuel/air equivalence ratio (ϕ), ignition timing (IT), engine speed (rpm) and EGR%. In order to allow distinction of the individual effects of these parameters, without resorting to a lot of one factor at a time sweeps, the experimental conditions have been chosen in such a way that Response Surface Methods can be applied to analyze the results [22]. This way, the resulting quantities of interest (e.g. IMEP, ignition delay) can be fit as a function of the individual parameters.

Model setup and calibration

As the main focus of the current work was to evaluate combustion models, the employed engine model is limited to the closed part of the engine cycle (IVC to EVO). The initial conditions for mass fractions of air and fuel, the mean temperature and pressure at IVC are taken from the measurements.

The residual gases (from the previous engine cycle) are estimated using a gas dynamics model of the entire intake and exhaust geometry constructed using the commercial engine simulation software GT-Power [6] in combination with measured valve discharge coefficients. Measured cylinder wall temperatures were applied to the cylinder wall, head and piston surfaces [23]. The heat transfer was calculated using the model of Woschni and the unburned mixture was treated as a single zone.

The calibration fixes the coefficients for the heat transfer model, the flame development model (C_1) and the turbulent burning velocity model (C_2;C_3). For each model, the code has been calibrated at the condition in the middle of the explored parameter space. The calibration constants are left constant for the other conditions.

Validation of the engine model

To evaluate whether the different turbulent combustion models can recover the correct behavior with the rms turbulent velocity u', residual ratio and engine geometry, experiments with varying engine speed (u) and external EGR% (residual ratio) have been performed on the Audi engine. Additionally variations in throttle position and ignition timing were considered according to Response Surface Methods.

The results are synthesized into graphs showing ignition delay (0-2% burn time), main combustion duration (10-90% burn time) and the IMEP error during combustion. These figures display sectional views at the center point (2500 rpm, IT=10 °ca BTDC, TP=50°, ϕ=1.0) of the response surfaces fitted to the experimental and simulation results. The results using the CFM and Gülder model are not presented here. The former because of its poor overall performance and the latter because of its resemblance to the Zimont model. Calibration constants are listed in Table 2.

u_t model	$C_{htr,\ compr}$	$C_{htr,comb}$	$C_{htr,exp}$	C_1	C_2	C_3
Damköhler	1,3	2,0	0,3	1,5	1,50	0,8
Zimont	1,3	2,0	0,3	1,5	0,38	0,8
Dinkelacker	1,3	2,0	0,3	1,5	0,45	1,0
Bradley *KaLe*	1,3	2,0	0,3	0,5	0,62	1,0

Table 2. Calibration constants for methanol operation

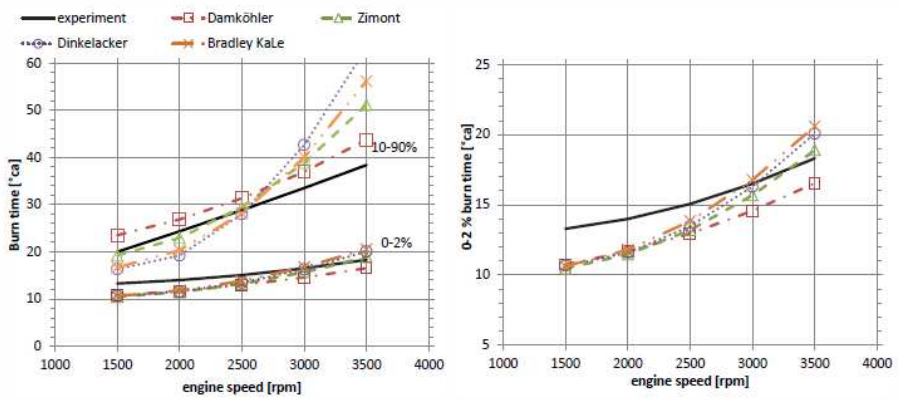

Figure 2. Comparison of u_t correlations for varying engine speed

Results for varying engine speed are plotted in Figures 2 and 4. For this engine model, the k − ε turbulence model of GT-Power was used in combination with the boundary conditions for u' and L obtained from a TPA analysis [8]. Figure 2 indicates that the Damköhler model better reproduces trends with u'. The u_{te} predicted by this model is more dependent on u' compared to the other formulations considered here (Eq. 1, $u_{te} \sim u'$). The Dinkelacker model performs worst since it is the least sensitive to changes in u' (Eq. 5, $u_{te} \sim Re^{0.25}u'^{0.3} \sim u'^{0.55}$). Then again, with the current research equipment it is impossible to verify whether the values for u' and L predicted by the employed turbulence model correctly reflect the real evolution with engine speed. Because the default turbulent combustion model in GT-Power is of the Damköhler type, the turbulence routines are possibly tuned for best performance with this model. Additionally, the influence of bulk flow motion (e.g. swirl, tumble) has been neglected.

Figures 3 and 4 illustrate the trends with varying ignition timing. As mentioned before, two effects are at play. On the one hand turbulence relaxes closer to top dead center (later ignition), reducing the combustion rate. On the other hand, the higher temperatures and pressures make for a higher initial laminar burning velocity.

The experimental ignition delay slightly reduces with retarded ignition timing, while all models predict a more pronounced variation. For the main combustion duration all models correctly reproduce the experimental trend. The IMEP error during combustion is limited to 0.25 bar.

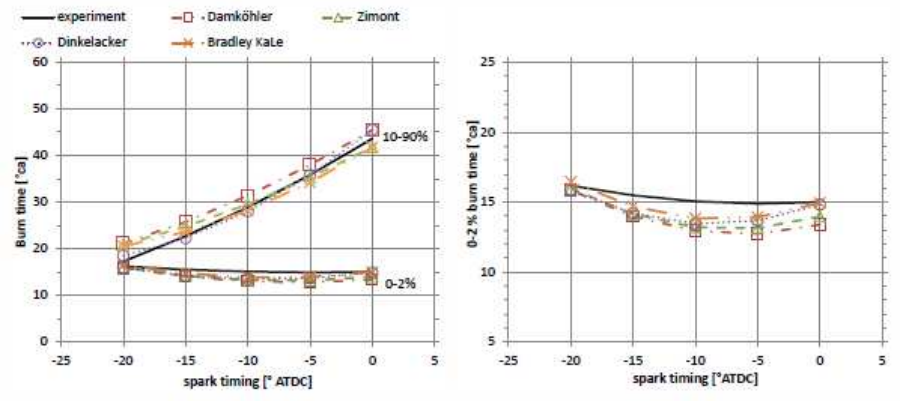

Figure 3. Comparison of u_t correlations for varying ignition timing

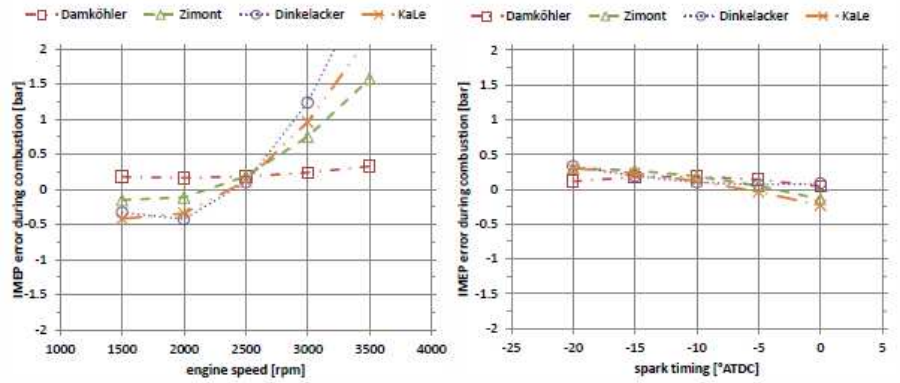

Figure 4. Comparison of u_t correlations for varying engine speed (left) and ignition timing (right)

For the effect of ϕ, the conclusions are similar as in the previous section (Figures 5 and 7). There is a slight overestimation of the 0-2% and 10-90% burn times for the richest mixtures by all models, except that of Dinkelacker, due to its strong dependence on Le. This strong dependence also causes overestimations of the main combustion duration for lean mixtures.

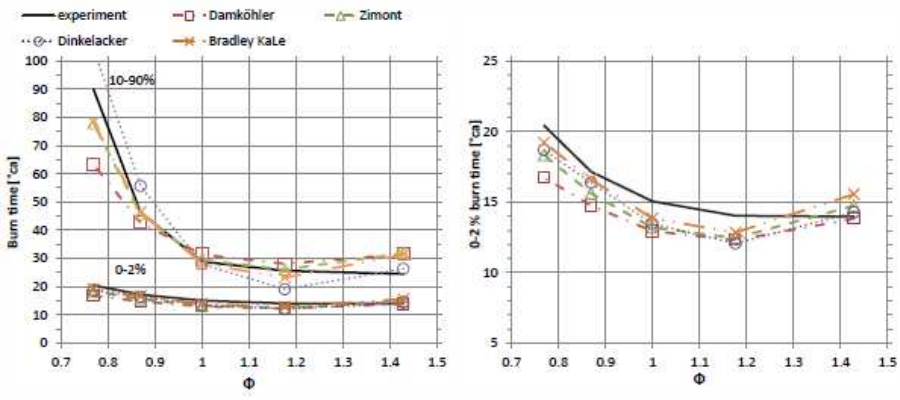

Figure 5. Comparison of u_t correlations for varying mixture equivalence ratio

The Zimont and KaLe expressions perform well, except for the leanest mixture, where there is a slight underestimation of the main combustion duration. It must be noted that this operation point was significantly affected by cycle-to-cycle variations (>30%) which compromises the reliability of the experimental results. The underprediction is even worse for the Damköhler model due to its low u_l sensitivity.

Figures 6 and 7 summarize the data for varying load. Reducing the load (throttle closer to 90°) has two effects in the simulation model. The turbulence is weaker due to less kinetic energy originating from the main flow and the

laminar burning velocity decreases as a result of increasing internal EGR levels. Although all models reproduce the correct trend, they underestimate the increase in ignition delay and 10-90% burn time with reducing load. This can be due to uncertainties in the estimation of turbulence and internal EGR obtained from breathing cycle simulation. The explicit pressure dependence in the expression of Dinkelacker (Eq. 5) leads to an overestimation of the effect of reduced load (~ reduced pressure).

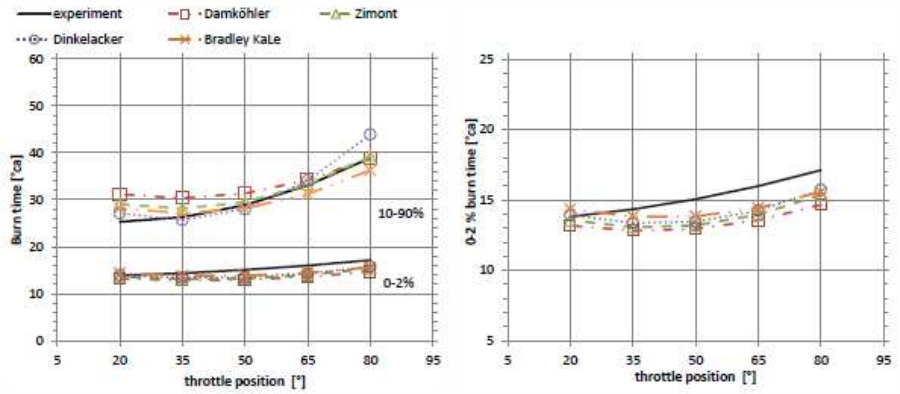

Figure 6. Comparison of u_t correlations for varying load (throttle position)

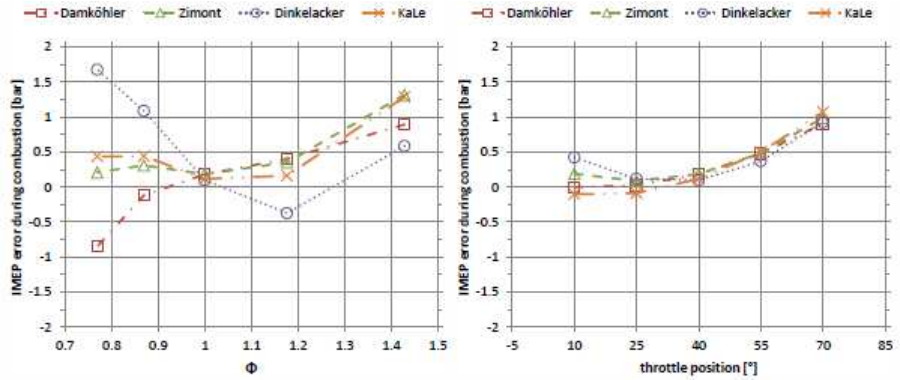

Figure 7. Comparison of u_t correlations for varying mixture equivalence ratio (left) and varying load (right)

Finally, the influence of external EGR on ignition delay and 10-90% burn time is illustrated in Figure 8. Because of the challenges associated with the control and measurement of EGR%, this factor was not included in the Response Surface Method dataset. Instead, some measurement points associated with the evaluation of alternative load control strategies are considered. These were obtained at 1500 rpm, wide open throttle, optimal spark timing and with varying amounts of EGR%.

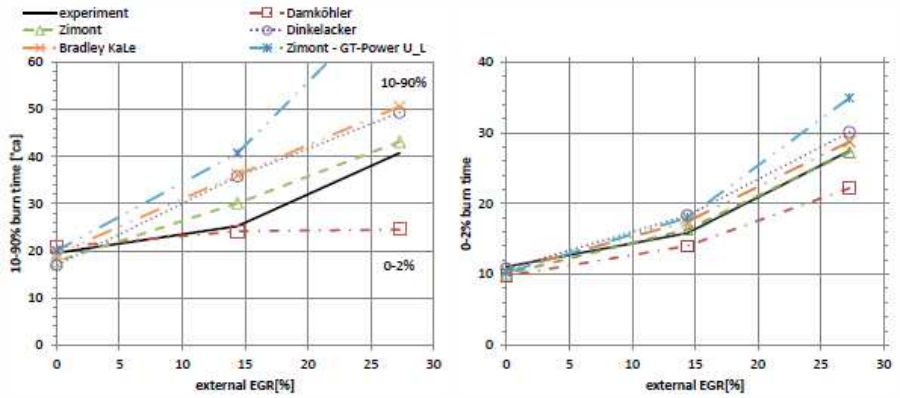

Figure 8. Comparison of u_l and u_t correlations for varying amounts of external EGR

Next to the different turbulent combustion models, the predictive performance of the default methanol u_l correlation in GT-Power (in combination with the Zimont u_{te} model) is tested. The residual gas term in this correlation is that of Rhodes and Keck [24] developed for gasoline. For the ignition delay, all models employing the new u_l correlation produce acceptable results. The Damköhler model underpredicts the effect of EGR

because of its relative insensitivity to u_l. The Rhodes and Keck residual gas term produces a too steep decline in u_l with higher EGR levels, leading to an overestimation of the ignition delay.

With regard to the main combustion duration, the respective over- and underpredictions by the Rhodes and Keck residual gas term and the Damköhler u_{te} model are even more marked. The turbulent burning velocity expression of Zimont produces the best results among the considered models. It must be noted that the simulation results are very sensitive to the EGR%. Both estimated internal EGR% and measured external EGR% are subject to absolute errors in the order of 1-3%. This makes it difficult to draw firm conclusions regarding the relative performance of the different turbulent combustion models. Further validation regarding the effect of residuals on combustion and possible cross-effects of temperature and ϕ remain desirable.

SUMMARY

The power cycle routines of the developed QD simulation code were validated against a database of cylinder pressure traces obtained for both methanol and ethanol operation, and varying engine speed, throttle position, ignition timing and equivalence ratio. The new laminar burning velocity correlations were shown to predict the effects of varying equivalence ratio much better than existing correlations. A comparison confirmed that turbulent burning velocity models including thermodiffusive properties (e.g. Zimont, Bradley KaLe) performed better than simpler formulations (e.g. Damköhler). The inclusion of a pressure dependent term in the turbulent burning velocity model of Dinkelacker led to poor predictions for varying throttle position and ignition timing.

Additionally it was found that the effect of engine rpm was best predicted by the Damköhler model, but this could be due to uncertainties regarding the turbulence levels inside this engine. Combining of the new u_l correlation with the turbulent combustion model of Zimont produced acceptable results for varying external EGR%, but further validation of this factor remains desirable.

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