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## 2<sup>nd</sup> Symposium on Ammonia Energy

### OD Simulation of NH<sub>3</sub> Combustion Based on Reaction Kinetics

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#### Combustion Applications (GT, ICE, Burners)

##### Introduction

Ammonia is being taken more and more seriously as an energy carrier for large marine vessels and off-highway use from year to year. Especially applications with high demands for power and energy density can profit from the use of an ICE rather than fuel cells or purely electric power storage. For an efficient application of ammonia in combustion engines, more basic mixing and combustion phenomena have yet to be understood and looked at with test bench measurements. However, for a later adoption of existing engine designs or the adoption of new engine models to ammonia combustion, simulation is equally needed. It helps to front load the design processes and is critical for an efficient dimensioning of the engine components and peripherals. To allow this, the intrinsic fuel properties of ammonia have to be gathered and processed in a way that they can be easily accessed by the simulation environment. Some of those properties, like the lower heating value or the stoichiometric air requirement are easy to implement. Others require reaction kinetic calculations and more effort to efficiently store and access – especially the laminar burning velocities and ignition delay times need extensive attention. For this, an automated methodology that acquires and stores up to 20 relevant fuel properties for pure fuels and especially fuel mixtures has been developed and presented in [1]. The aim of this work is to validate the already established process for its application in ammonia combustion.

##### Materials and Methods

With the established process, laminar burning velocities are calculated by the means of the Cantera [2] reaction kinetic software and the Stagni [3] kinetics mechanism. To gather data for all relevant engine conditions, an adiabatic free flame calculation is done for a wide range of boundary conditions. As this creates a five-dimensional array with at least 50,000 entries, a multiprocessing method is utilized. This allows for multiple parallel function calls and good scaling with additional processing units. The dimensions of the result data are also challenging when they need to be accessed during the engine simulation itself. A single cycle in 0D/1D working process calculation needs less than a tenth of a second in solving time. During one of these cycles, the laminar burning velocity is read for each calculation step, roughly at least a hundred times per cycle. To guarantee fast access times while keeping the accuracy, a mathematical correlation is implemented. It is derived from the works of Mueller [4], and was then extended by Ewald [5], Hann [6], and the author of the present work [1]. It is based on Equation (1) with additional equations for the frequency factor  $A_{T,0} = f(\phi, w_{EGR})$ , the reactive mass fraction  $w_r = f(T_0)$ , the temperature of the inner layer  $T_0 = f(T_{ub}, \phi, p)$ , and the burned temperature  $T_b = f(T_{ub}, w_{EGR}, \phi)$ . The boundary conditions are defined by the pressure  $p$ , the unburnt temperature  $T_{ub}$ , the fuel/oxidizer equivalence ratio  $\phi$ , and the recirculated exhaust gas ratio  $w_{EGR}$ . Optionally, the external water ratio  $w_{H_2O}$  can also be addressed. A total of 12 correlation parameters and 4 spline tables exists. They are all automatically fit to the reaction kinetic calculation results in a distinct order. Details on the exact fitting process can be found in [1].

$$s_L = A_{T,0} \cdot w_r^m \cdot \left(\frac{T_{ub}}{T_b}\right)^r \cdot \left(\frac{T_b - T_0}{T_b - T_{ub}}\right)^n \quad (1)$$

For the validation of the simulation results, burn rate curves are utilized. They are generated by a three pressure analysis (TPA) done for measurements on a single cylinder research engine with a displacement of 500 cm<sup>3</sup> and a stroke-to-bore ratio of 1.035 as fully described in [7]. Overall, 54 operation points with variations of engine speed, engine load, equivalence ratio, and spark timing have been evaluated. Unfortunately, there was no information available on the cylinder head flow characteristics of this specific engine geometry, so the parameters for the swirl/tumble and turbulence models had to be estimated. Additionally, the wall heat model has been only roughly dialed in due to time constraints. The effects of these uncertainties will be noticeable when comparing the simulation results to those of the TPA. The calibration of the combustion model was done for a low-load, low-speed operating point.

## Results and Discussions

In the following, burn rate comparisons for a load and an equivalence ratio variation at 3000 rpm engine speed are made. For the load variation in Figure 1, both measurement data and simulation show a great agreement, the trend in the load variation is well met. Slight deviations occur at the beginning and the end of combustion.

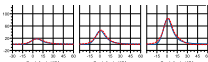


Figure 1: Load variation at 3000 rpm for ammonia fuel. Simulated burn rates vs. TPA-results.

The equivalence ratio variation in Figure 2, almost shows the same accuracy. The lean operation point at  $\lambda = 1.29$  reveals higher deviations, the curves shapes and their covered area

indicate that not the same amount of energy is converted. In this case, the difference is not caused by inaccuracies in the fuel data but has to be affected by other simulation parameters or an inexact TPA model/process.

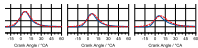


Figure 2: Equivalence ratio variation at 3000 rpm and 8 bar load. Simulated burn rates vs. TPA results.

When looking at the predicted IMEP results for all operating points that were dealt with in Figure 3, two kinds of deviations can be observed: First, all simulated operating points are

prone to underpredict the indicated mean effective pressure. A slightly underestimated thermodynamic compression ratio, a miscalibrated wall heat transfer model or general deviations in the TPA model could cause this effect. Additionally, at the operation points for 8 and 15 bar load, smaller clusters form. Here, deviations above and below the bisecting angle are observed. At these operating points, the spark ignition timing has been varied. Currently it is assumed, that the extremely early combustion starts are causing errors as the early phase of combustion is not properly met. If more data about the cylinder head and the valvetrain was known, uncertainties could be identified and eliminated.



Figure 3: Congruence between the simulation and TPA results for the prediction of the mean indicated effective pressure

Then both these issues could be quantified, judged, and possibly ironed out. Nevertheless, the current quality of the simulation model suggests that the established workflow also is applicable

for ammonia combustion.

## Conclusions

It has been shown, that the presented toolchain and its results are capable of accurately describing ammonia combustion. This is validated for engine load, engine speed, and enleanment sweeps. Due to smaller inaccuracies in the simulation model description, the results for predicted mean effective pressures are slightly offset to the measurement values. A reevaluation of the model inputs and measurement data should be able to resolve this.

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