

NUMERICAL AND EXPERIMENTAL STUDIES OF KNOCK IN DUAL-FUEL ENGINES

S.C. Li, H. Li and F.A. Williams
Center for Energy and Combustion Research
University of California, San Diego
La Jolla, CA 92093

K. Gebert
BKM Inc.
San Diego, CA 92109

ABSTRACT

The present paper reports numerical and experimental results concerning knock in dual-fuel engines, where liquid diesel fuel is used as an ignition source to ignite a combustible mixture of natural gas (NG) with air.

A diesel engine (Caterpillar 3406B) was converted to a dual-fuel configuration which included an advanced pilot diesel-fuel injection system, a multipoint sequential gas-injection system and an accurate engine electronic control module. The engine was tested with a mass ratio, R_p , of diesel to NG less than 5%, and an equivalence ratio, Φ , of the NG-air mixture less than 0.6 and compression ratio is 15. The maximum cylinder pressure was up to 140 bar in the present experiment. Cylinder pressures were recorded by a transducer which had a natural frequency high enough to respond to typical knock pressure vibrations ranging from 4 to 10 kHz. The unfiltered signal was monitored by an oscilloscope and a computer. The crank angle, θ_k , at which knocking starts in the cylinder, can be determined from pressure signals. Knock occurrence also was recorded using a Bosch piezoelectric vibration sensor mounted on the cylinder head. Experiments demonstrated that the dominant factors influencing knock occurrence for a specified compression ratio are θ_i , the crank angle at which the premixed flame starts to propagate, T_0 , the intake temperature of the NG-air mixture, Φ and R_p . It was also found that if knock does not occur by the time that the highest cylinder pressure is reached, then it does not occur at all.

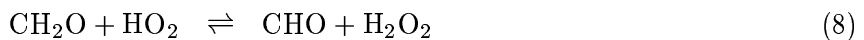
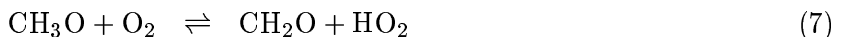
In order to model preknock chemical processes, the combustion chamber was divided into two zones separated by the propagating flame, namely the end-gas zone and the product zone. Knock

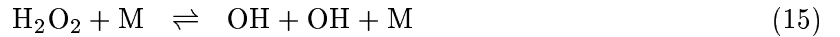
is treated as explosion of the combustible gas mixture in the end-gas zone, produced by the heating associated with the rapid increase of cylinder pressure. Numerical computations are thus simplified by reduction of the applicable conservation equations to a set of stiff ordinary differential equations that describe histories of temperature and species concentrations of the end-gas zone. This initial-value problem is solved by the Gear method with an internally generated full Jacobian matrix. The present study employs a detailed C₁-C₂ mechanism consisting of 102 elementary reactions among 26 species. This reaction mechanism is derived from our earlier 177-step reaction mechanism [1] by deleting C₃ species (reactions 100-125) and nitrogen chemistry (reactions 126-177) and adding three reactions, $\text{CH}_4 + \text{O}_2 \rightleftharpoons \text{CH}_3 + \text{HO}_2$, $\text{CH}_4 + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}_2$ and $\text{CH}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{CHO} + \text{H}_2\text{O}_2$ with their rate parameters being taken from the paper by Leung and Lindstedt [2] (reactions 80, 122 and 123).

Sensitivity analysis shows that 12 species are most important in preknocking chemistry in dual-fuel diesel engines with equivalence ratio $\Phi < 0.6$, namely, O_2 , OH , HO_2 , H_2O_2 , H_2O , CH_4 , CH_3 , CH_3O , CH_2O , CHO , CO and CO_2 . The most important initiation reactions at end-gas temperatures below 900 K were found to be



In this temperature range, other reactions are much slower. For higher end-gas temperatures up to 1100 K (near the highest temperature at which knock may start), reactions 1 and 2 become unimportant, and reactions 3 and 4 are accompanied by the following twelve reactions:





These 16 elementary reactions can be used as a starting preknock chemistry to provide a basis for a reduced reaction mechanism in predicting knock phenomena in dual-fuel diesel engines.

Typical results of experiments and numerical computations are plotted in Figs. 1 and 2 where influences of T_0 and θ_i on knock are shown under the same Φ , R_p and compression ratio. Predicted end-gas temperature histories are plotted in Figs.1(a) and 2(a) according to the full reaction mechanism (102 elementary steps) and the 16-steps starting preknock chemistry described above. In these figures, knock starts as the end-gas temperature runs away. Figure 1(a) indicates that higher intake gas temperature, T_0 , leads to an earlier and sharper temperature rise. Knock does not occur when T_0 is low enough. These results clearly demonstrate that the end-gas temperature plays an important role in preknock reactions in the end-gas zone. Figure 2(a) illustrates how θ_i influences the end-gas temperature history shows that earlier ignition of the NG-air mixture (more advanced θ_i) results in an earlier and sharper temperature surge. The end-gas temperature does not run away if θ_i is retarded enough. These results are consistent with the observation that the cylinder pressure begins to increase earlier when ignition of the NG-air mixture occurs earlier and, consequently, the end-gas temperature starts to rise earlier. Figures 1(b) and 2(b) plot measured and computed values of θ_k , the knock-occurrence crank angle, as a function of T_0 and θ_i , respectively. several conclusions can be drawn from these figures. First, higher intake gas temperature and earlier ignition of the NG-air mixture lead to earlier and stronger knock. Second, predicted knock occurrence agrees well with the available measurement. Third, predicted knock occurrences with the 16-step preknock chemistry is essentially the same as that with the full reaction mechanism.

In summary, a starting reaction mechanism has been developed for predicting knock occurrence in dual-fuel diesel engines. The present work help to identify the most important species and reactions which lead to knock. Good agreement was found between numerical predictions and experimental results for one particular engine, suggesting that the present 16-step reaction mechanism, implemented in CFD codes, may predict knock phenomena well in lean premixed dual-fuel engines.

References

- [1] Li, S.C. and Williams, F.A., "NOx Formation in Two-Stage Methane-Air Flames," *Combust. Flame*, Vol.117, to appear, 1999.
- [2] Leung, K.M. and Lindstedt, R.P., "Detailed Kinetic Modeling of C₁-C₃ Alkane Diffusion Flames," *Combustion and Flame* 102:129 (1995).

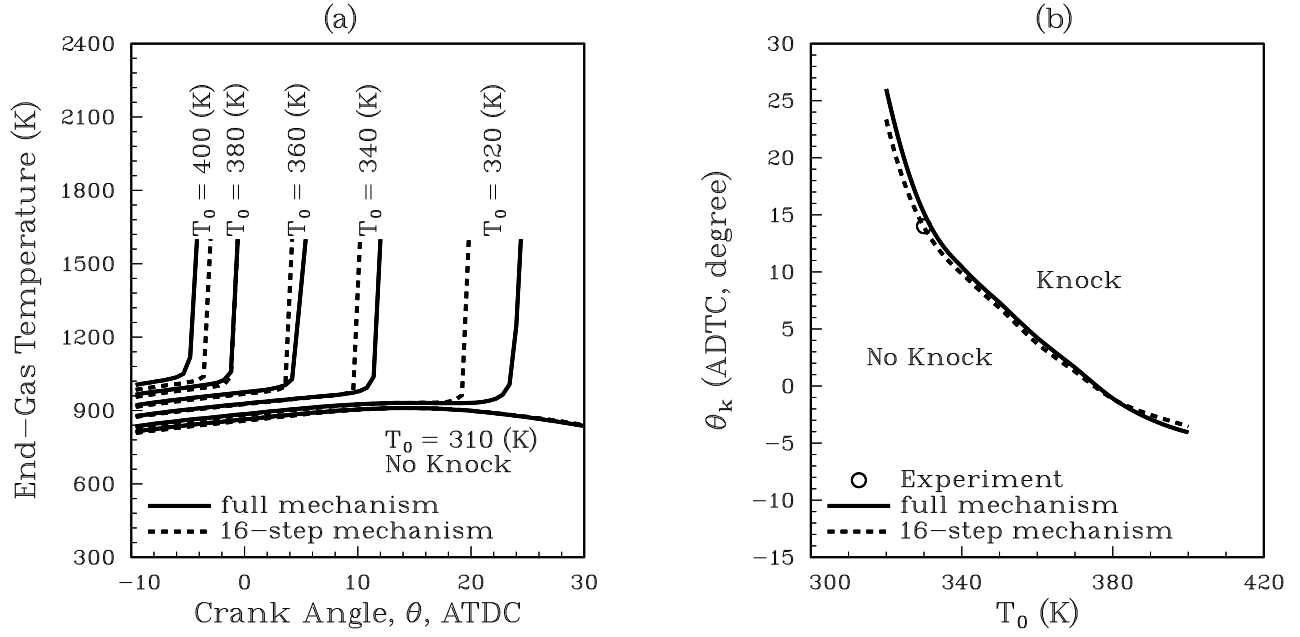


Fig.1: Influence of intake-gas temperature (T_0) on knock in a dual-fuel diesel engine with $\Phi = 0.561$ and $\theta_i = -10^\circ$: (a) End-gas temperature history at different T_0 ; (b) Dependence of knock occurrence θ_k on T_0 .

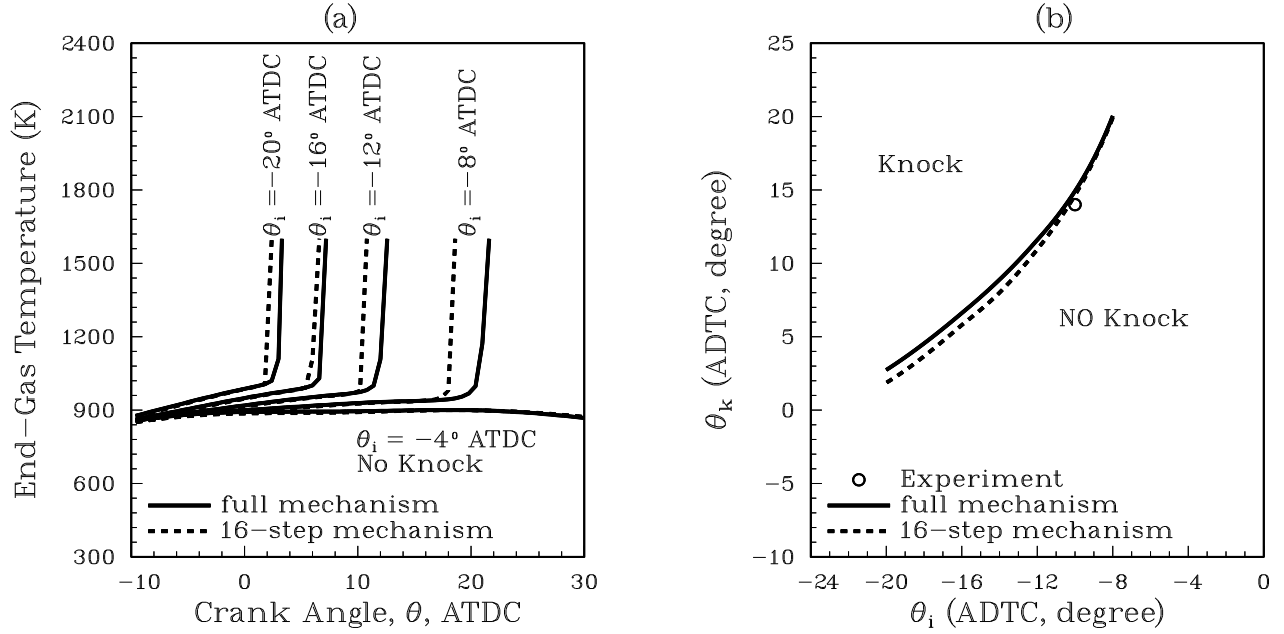


Fig.2: Influence of ignition timings (θ_i) on knock in a dual-fuel diesel engine with $\Phi = 0.561$ and $T_0 = 300$ K: (a) End-gas temperature history at different θ_i ; (b) Dependence of knock occurrence θ_k on θ_i .