

OPTIMISATION OF DIESEL AUTOIGNITION TABULATION PROCEDURES FOR AVL CODE "FIRE"

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Abstract. *The modifications of existing Diesel auto-ignition tabulation for CFD code AVL "FIRE" will be presented in this paper. Current n-heptane tabulation (used to simulate Diesel behaviour in IC engines) did not include the phenomenon of cool flame ignition. This phenomenon is important since the temperature of the air/fuel mixture is significantly higher after its occurrence and the simulation results could be improved if this is also taken into consideration when simulating combustion in Diesel engines.*

Current methods of auto-ignition computation in AVL FIRE are based on the extraction of ignition delay times from tabulated data dependent on four parameters: temperature, pressure, air excess ratio and EGR mass fraction. The new tabulation procedure was developed using the same parameters as starting points for two-step chemical combustion. Temperature changes were observed and a compilation of several criteria was used to determine the start of both cool flame and main ignition. The above parameters were varied and the calculations were performed for each parameter set. Chemical software was used for two-step combustion calculations, using reduced then complex chemical mechanisms, and the results of calculations were stored in a binary file. Results included the values for cool flame ignition delay, main ignition delay, and cool flame and main ignition heat releases.

This paper will present the methods used to determine the ignition delays (cool flame and main ignition), as well as results comparing the data acquired using three different chemical mechanisms (three levels of complexity). The data acquired from the calculations would be used to optimize the tabulation procedure using more complex (accurate) chemical mechanisms in a way which will also be described.

1 INTRODUCTION

Recent rapid advances in computer power lead to increased use of computational tools in engine design, significantly reducing the costs of simulations in comparison with engine experiments.

In addition, there has been significant improvement in the physical sub models used in engine simulations, and the enhanced accuracy has made the use of computational tools advantageous for generating a better understanding of the transient physical and chemical phenomena that occur in internal combustion engines. The goal of this study was to improve the prediction of diesel autoignition processes.

Flame development, power output and emissions formation are determined by the process of autoignition in Diesel engines and is dependent on chemical and physical processes. The first kind of processes are pre-combustion reactions of the fuel with air and residual gases, high temperature combustion and emissions formation. The main physical processes include atomization of liquid fuel, evaporation of fuel droplets and turbulent mixing of vapor with air. Rather than trying to simulate the complex behavior of diesel itself the replacement fuel of choice is n-heptane due to its cetane number of approximately ~56, which is similar to that of ordinary Diesel fuel¹.

Current diesel autoignition model included in AVL code "FIRE" used a tabulated data acquired by running SENKIN calculations varying following initial parameters: temperature, pressure, air excess ratio and recirculated exhaust gas mass fraction². These values were used to simulate the exact ignition moment using a precursor variable in extended coherent flame combustion model. However, existing data provides only the main ignition delays and this showed bad influence on results when running simulations in a low temperature region without taking cool flame phenomenon into account.

During the work described in this paper, the oxidation process of auto-ignition is calculated using CHEMKIN II code (and modified SENKIN subroutines), assuming zero dimension and adiabatic changes. Calculations were performed using three levels of chemical model complexity.

2 CHEMISTRY BACKGROUND AND NUMERICAL APPROACH

When studying the complex chemical mechanism, it is possible to get a comprehensive insight of the chemical kinetics behind the phenomena of autoignition. The complete complex reaction mechanism for n-heptane oxidation included 2450 elementary reactions among 550 chemical species³. The detailed n-heptane mechanism (of Curran et. al.) is intended to cover the entire range of conditions from low-temperature (600-900 K) pyrolysis and oxidation to high-temperature combustion.

N-heptane, which is a straight-chained fuel, is assumed to lead to alkenyl decomposition products with alkyl radicals and olefins. Due to the comprehensive mechanism of n-heptane oxidation, n-heptane molecules undergo H-atom abstraction at high and low temperatures, leading to the formation of structurally distinct alkyl radicals. When alkane fuels have to stay partially or fully premixed in an oxidizing atmosphere at elevated temperatures and pressures,

ignition can occur in a multistage mode. The ignition process can follow completely different schemes of oxidation and is controlled by two different chain-branching reaction mechanisms: the low-temperature reaction path, where the fuel is oxidized by O_2 in degenerated branched chains, and the high-temperature path, where the fuel is rapidly oxidized into C_2 and C_1 hydrocarbons and subsequently consumed. The low-temperature branch is quite complex and proceeds via different sub mechanisms, which are sensitively controlled by temperature.

At high temperatures, reaction processes via radical β -scission lead to smaller olefins and other radical species. At low and intermediate temperatures (600-900 K), peroxide chemistry becomes more important. The n-heptyl radical reacts with molecular oxygen, $R + O_2 = RO_2$, forming a heptylperoxy radical ($C_7H_{15}OO\cdot$). After the internal H-abstraction, the radical undergoes a second addition of O_2 forming hydroperoxy-heptylperoxy radicals, which are very unstable and decompose easily. Its products are both chain propagating and degenerating branching agents.

In this autoignition study, a FORTRAN code called SENKIN was used. It is generally used to predict the time-dependent kinetics behaviour of a homogenous gas mixture in a closed system using the set of CHEMKIN supplied routines. There are many possibilities for the chemical kinetics problems that one may need to solve for various applications. In Senkin there are six problem types that could be solved. The distinction between the problems comes from the externally imposed thermodynamic conditions⁴. The problems interesting to this study are:

- an adiabatic system with constant pressure,
- an adiabatic system with constant volume.

The energy equation for the constant pressure case is

$$c_p \frac{dT}{dt} + v \sum_{k=1}^K h_k \dot{\omega}_k W_k = 0, \quad (1)$$

where the mean specific heat of the mixture is $c_p = \sum_{k=1}^K Y_k c_{p,k}$. The net chemical production rate $\dot{\omega}_k$ of each species results from a competition between all the chemical reactions involving that species. Each reaction proceeds according to the law of mass action and the forward rate coefficients are in the modified Arrhenius form⁵

$$k_f = AT^\beta \exp\left(\frac{-E}{RT}\right), \quad (2)$$

where the activation energy E , the temperature exponent β , and the pre-exponential constant A are parameters in the model formulation.

Since monitoring the cool flame phenomenon was one of the main topics of this work, a way to create a general routine to be able to recognize both the cool flame and main ignition had to be created. A useful definition of the ignition delay time was obtained from Marakides which states that it could be presented as the time at which the temperature theoretically becomes infinite⁶ (the asymptote of the temperature curve – see Figure 1).

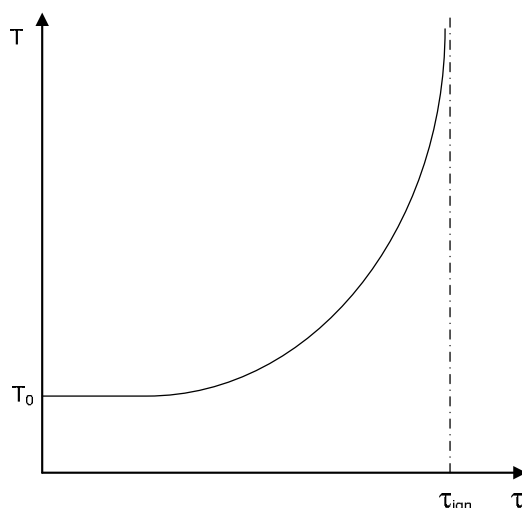


Figure 1: Simple theoretical ignition delay definition

Several other criteria had also be implemented on top the SENKIN code to make it possible to get both the cool flame and main ignition delay times and to filter out the misleading ignition candidates at the beginning of the calculation and around 1000 K. After each time step a temperature gradient is checked and if an inflexion occurs the time is stored to a vector variable. At the end of the calculation if there is only one record in the vector variable no cool flame ignition had occurred. In other case the first record is taken to be the cool flame ignition delay, and the last one is main ignition delay.

Three different chemical mechanism have been compared:

- simple *Golovitchev* with 59 species and 291 reactions (*simple* in further text),
- reduced *Curran et. al.* with 159 species, 770 reactions (*LLNL reduced* in further text) and
- complex *Curran et. al.* with 556 species, 2540 reactions (*LLNL complex* in further text).

Figure 2 shows that using *simple* mechanism one does get a two-stage ignition but the values are highly underestimated. The other image shows the difference between the *LLNL* mechanisms with low and high initial temperatures thus showing that the *LLNL reduced* mechanism works well for low temperature ignition but under predicts at higher temperatures (assuming that *LLNL complex* mechanism is accurate both at low and high temperatures).

However, it is still considerably better than *simple* mechanism.

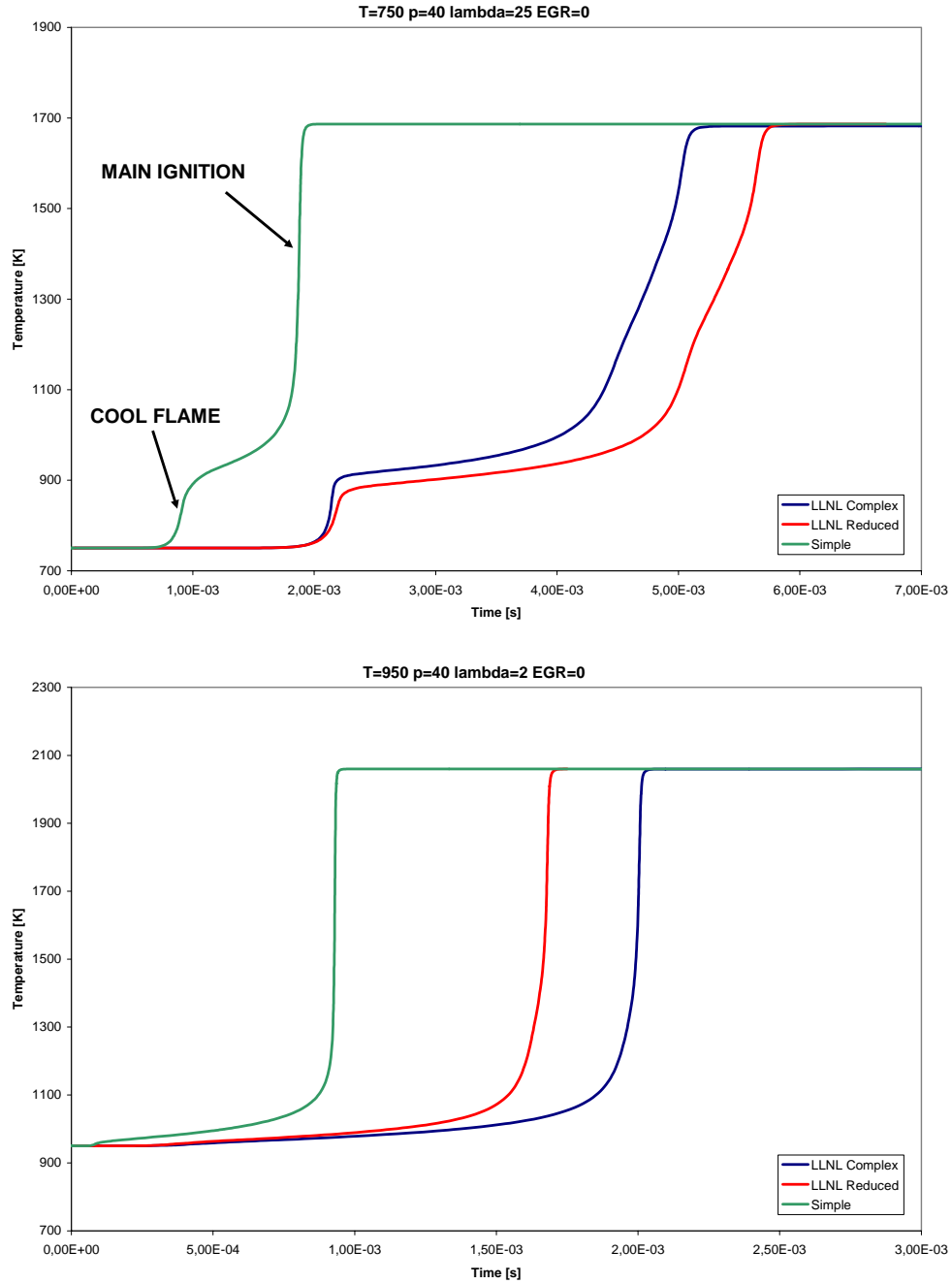


Figure 2: Mechanisms comparison for two initial parameter sets

3 CALCULATION SETUP

The ignition data tables should have provided the following data: cool flame ignition delay, cool flame heat release, main ignition delay and main heat release. Initial parameter ranges were taken out of existing tables (consisting of only main ignition delay times) and are shown in Table 1.

Temperature [K]	600 - 1500 (20K step)							
Pressure [bar]	10	15	20	25	30	40	60	80
Air excess ratio [-]	0.3	0.5	0.7	1	1.5	3		
EGR [%]	0	0.3	0.6	0.8				

Table 1 : Initial data

To acquire the needed data on the whole domain the total number of calculations is $45 \times 8 \times 6 \times 4 = 8640$. Computer used for the calculations had 2 dual-core Xeon EMT64 processors and 2Gb of RAM, and the average times to finish one ignition calculation are shown in Table 2.

Mechanism	Time
<i>simple</i>	25 min
<i>LLNL reduced</i>	2,5 hour
<i>LLNL complex</i>	2,5 day

Table 2: Average calculation times

Multiplying the average calculation time with the needed number of calculations clearly shows a need for another approach for getting the ignition data throughout the domain of interest using complex models. The full calculation sets were done using *simple* mechanism and lasted for around 5 weeks (4 simultaneous calculations). The data stored in a binary file as a 5 dimensional matrix was then used for visualization and comparison with complex models as well as for determining the further steps.

4 SIMPLE MECHANISM CALCULATION RESULTS

Following images show tabulated ignition delay data in 3D charts. Parameters held constant for each image were EGR mass fraction and air excess ratio. The idea behind this way of displaying data is to find the areas of near linear dependence of ignition delays on temperature and pressure to reduce the number of necessary calculations. Using the *LLNL reduced* mechanism (agreed on the fact that results it provides are close enough to the *LLNL complex* mechanism), acceptable number of calculations would be under 3000.

For initial temperatures of over 800 K cool flame ignition was either very hard to detect or so close to the main ignition that there was no need to separate the two.

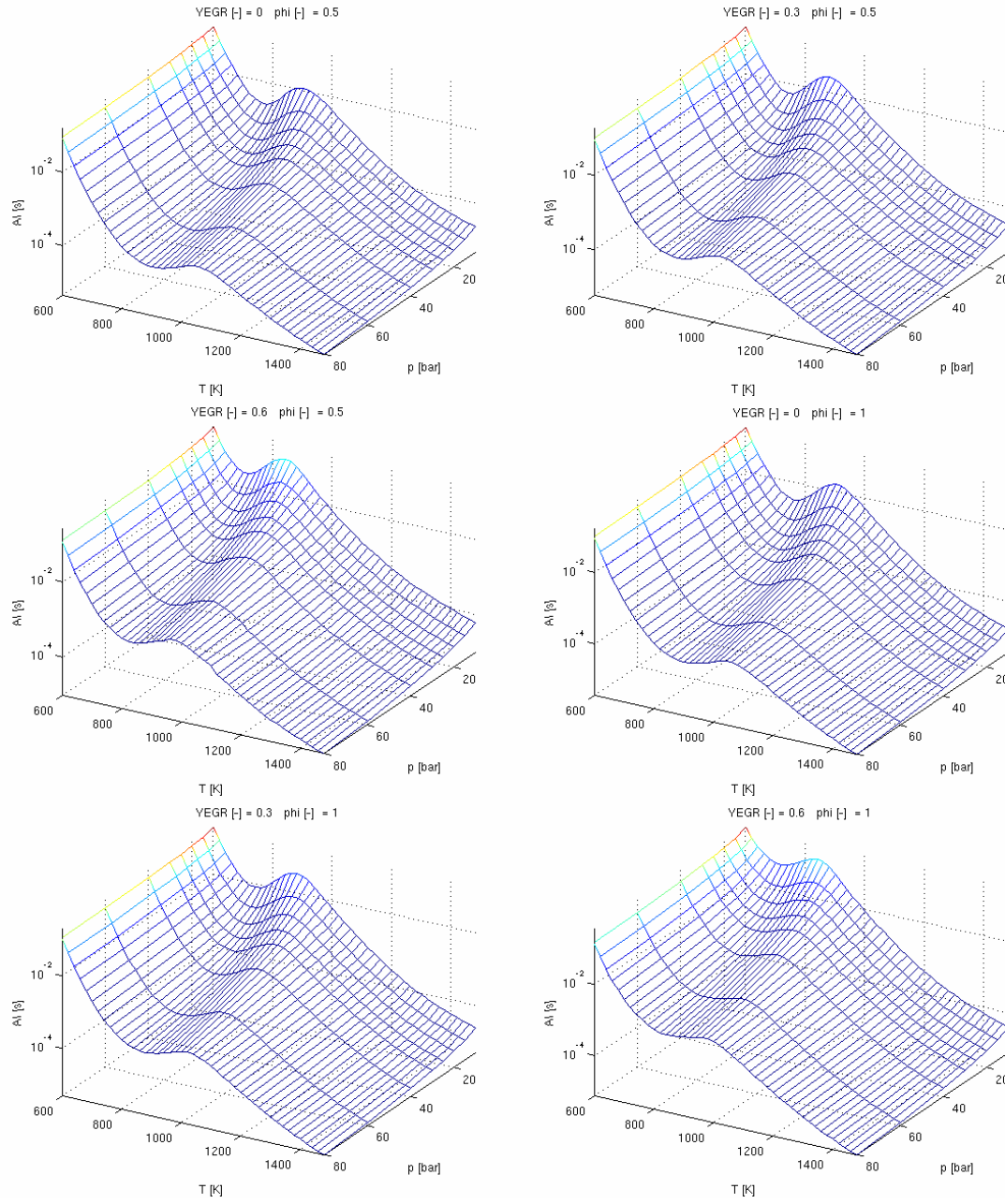


Figure 3: Main ignition temperature and pressure dependence

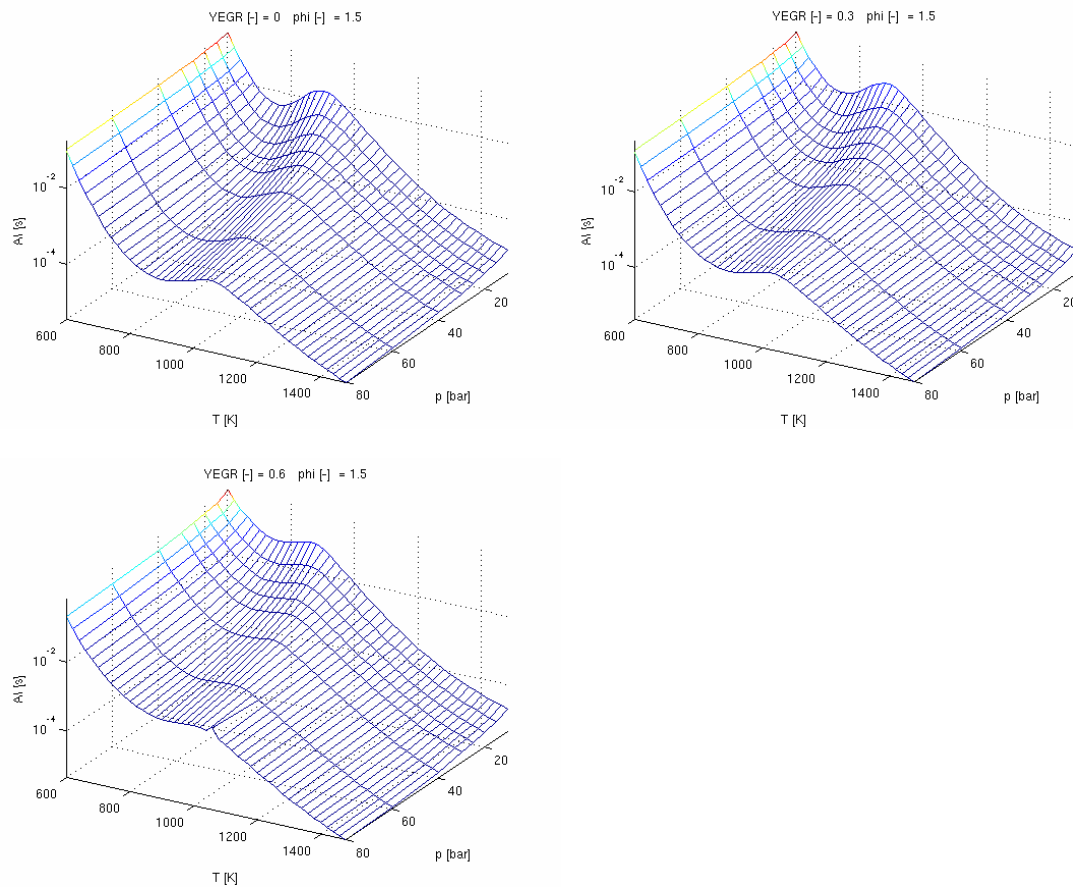


Figure 3 (continued): Main ignition temperature and pressure dependence

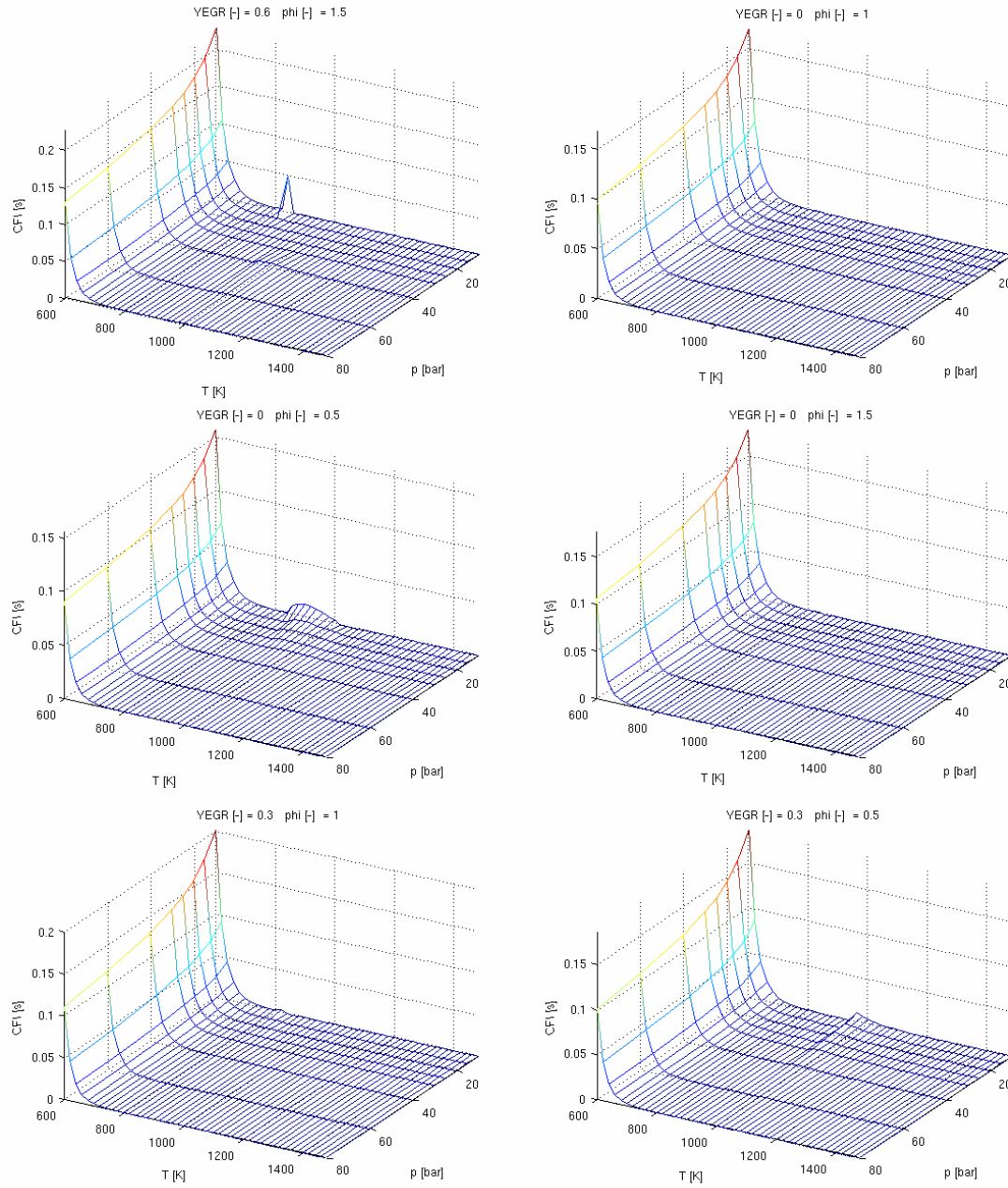


Figure 4: Cool flame delay temperature and pressure dependence

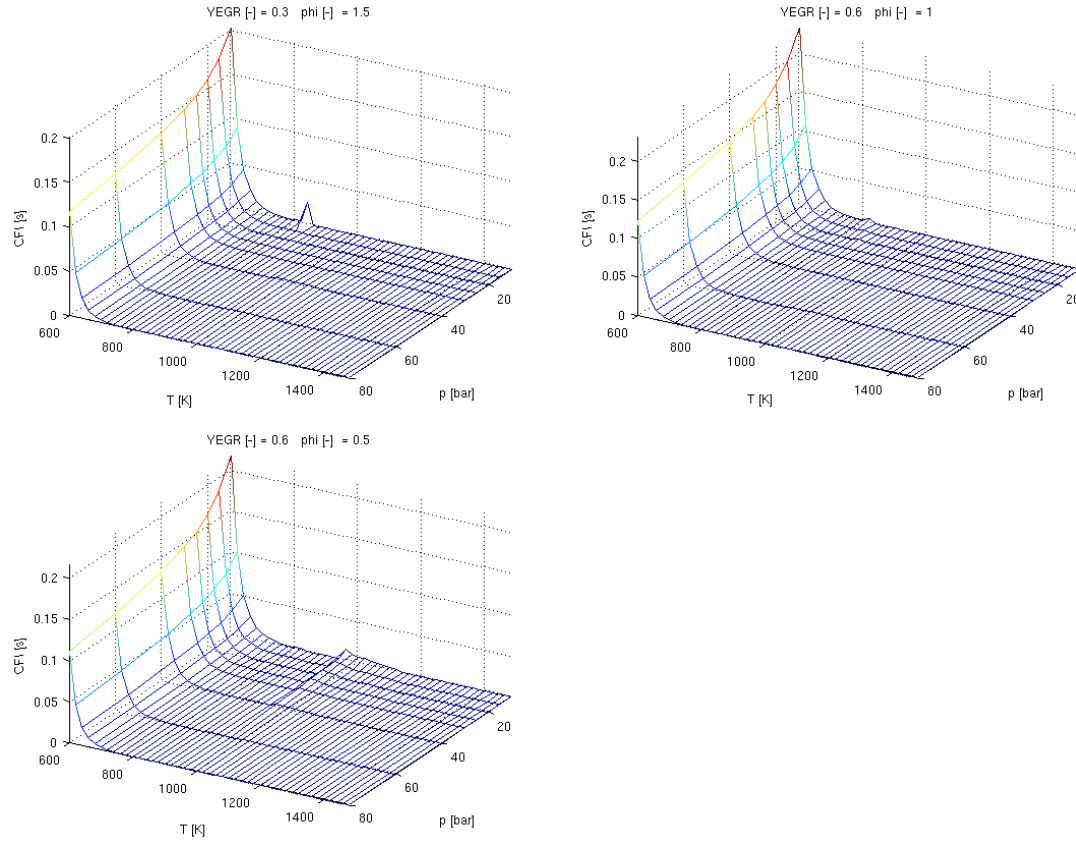


Figure 4 (continued): Cool flame delay temperature and pressure dependence

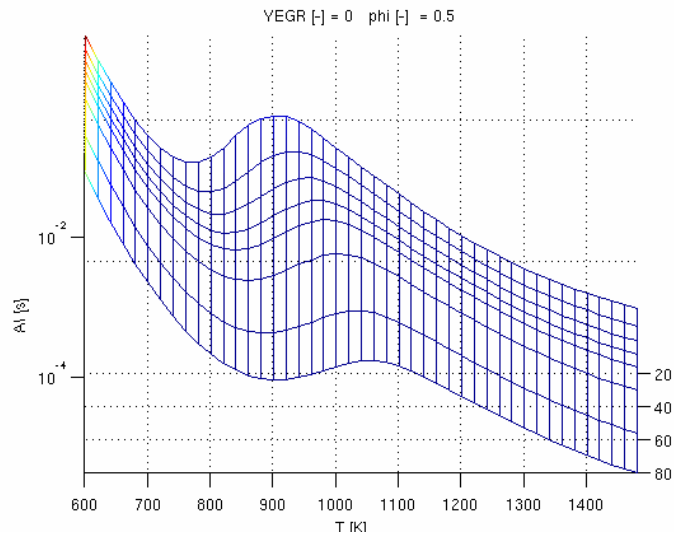


Figure 5: Main ignition temperature dependence

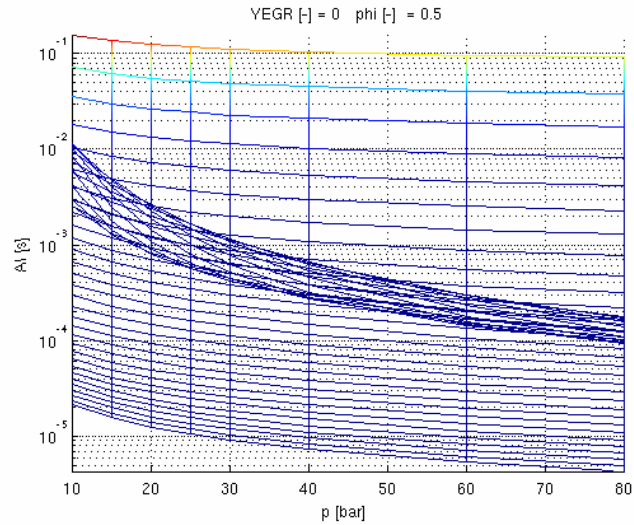


Figure 6: Main ignition pressure dependence

Figure 5 and Figure 6 (as well as the Figures 3 and 4) show that there is room for coarser distribution of temperature and pressure. There is no need for any temperature distribution points between 1100 K and 1500 K, as well as changing the distribution from 20 K to 40 K in other part of the temperature span. This would also catch the characteristic wave-like dependence in the low temperature area, and would reduce the number of calculations to only 2500. This is well inside the needed number of calculations but looking at the cool flame ignition delays, there is still a need to leave the initial temperatures with finer distribution in

the 600-750 K span. On the other hand, when looking at the pressure dependencies one can easily come to conclusion that there is no special need for all the lower range pressure points, thus compensating for finer low temperature distribution.

5 CONCLUSIONS

- *LLNL reduced* model should and will be used to create more accurate autoignition lookup tables (it represents the low temperature ignition delays far more accurately than *simple* mechanism)
- to obtain the tables in reasonable time the calculation domain (temperature and pressure) have been optimized
- new temperature distribution would be: 650 K – 750 K (20 K step), 790 K – 1110 K (40 K step) and 1500 K
- new pressure distribution would be: 10 bar, 20 bar, 30 bar, 80 bar
- new number of calculations would be: $14 \times 4 \times 6 \times 4 = 1344$, and would take (using the same computer power as earlier tabulation using *simple* mechanism) 35 days

REFERENCES

- [1] T.Rente *, V. I. Golovitchev, and I. Denbratt, *Numerical Study of n-Heptane Spray Auto-Ignition at Different Levels of Pre-Ignition Turbulence*, Thermo- and Fluid Dynamics, COMODIA 2001, 2001.
- [2] AVL LIST GmbH, AVL FIRE™, *CFD solver v8.3*, Graz, 2004.
- [3] H.J. Curran, P. Gaffuri, W.J. Pitz, and C.K. Westbrook, *A Comprehensive Modeling Study of n-Heptane Oxidation*, Combust. Flame 114 (1/2) (1998) 149-177.
- [4] A.E. Lutz, R. Kee and J. Miller, *Senkin: A Fortran program for predicting homogeneous gas phase chemical kinetics with sensitivity analysis*, Report No. SAND87-8248.UC-4, Sandia National Laboratories, 1987.
- [5] R. J.Kee, F. M. Rupley, J. A. and Miller, *Chemkin-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics*, Report No. SAND89-8009.UC401, Sandia National Laboratories, 1989.
- [6] C. N. Markides, *Advanced Autoignition Theory / Introduction*, Cambridge, 2004.