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Automatic Generation of Reaction Mechanisms for Description of Oxidation of Higher Hydrocarbons

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Abstract

Oxidation mechanisms even for rather simple hydrocarbons like heptane consist due to the occurrence of many isomeric structures of thousands of reactions of hundreds of species. The automatic generation of these reaction mechanisms using artificial intelligence means is described. Results are presented for *n*-heptane-air mixtures, where a hand-written reaction mechanism tested against experimental data is available.

1. Introduction

Auto-ignition processes play an important role e.g. in safety technology, in engine combustion (Diesel engine ignition, Otto engine knock) or in gas turbines. Typical temperatures for the occurrence of auto-ignition processes in hydrocarbon-air mixtures are between 600 K and 1000 K [1,2], showing the phenomenon of two-stage ignition [3] and negative temperature dependence [4-7], indicating a highly nonlinear behaviour.

At high temperatures ($T > 1100$ K at atmospheric pressure) combustion processes (e.g. flame propagation) occur via alkyl radical pyrolysis and subsequent oxidation of CH_3 and C_2H_5 [8,9]. At low temperature (e.g. in ignition) the fast radical pyrolysis is too slow to lead to the fuel-unspecific CH_3 and C_2H_5 oxidation. Thus, low temperature chemistry is very fuel-specific, and the large variety of isomeric structures of the large hydrocarbon structures occurring lead to complicated large reaction mechanisms with thousands of reactions of hundreds of species even for a fuel like heptane [10,11].

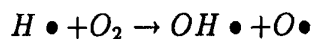
It is a very frustrating work to write down these large reaction mechanisms, and printing errors are easily made. Thus, computer aided generation of these mechanisms is described in this paper, avoiding these disadvantages and allowing the generation of huge reaction mechanisms necessary for the description of ignition and combustion e.g. of mixtures of large aliphatic hydrocarbons (or even gasoline in the long run).

2. Reaction Mechanism and Numerical Integration

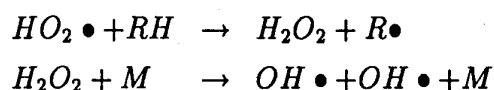
2.1 Reaction Mechanism

Ignition mainly is governed by chain branching processes which are rather unspecific of the fuel considered at high temperature, whereas they are fuel specific at low temperature, leading to very complex reaction systems if the numerous different isomeric structures are taken into consideration.

Chain branching at high temperature ($T > 1100$ K at $P = 1$ bar) is predominantly provided by ([8]; • is marking a radicalic site)



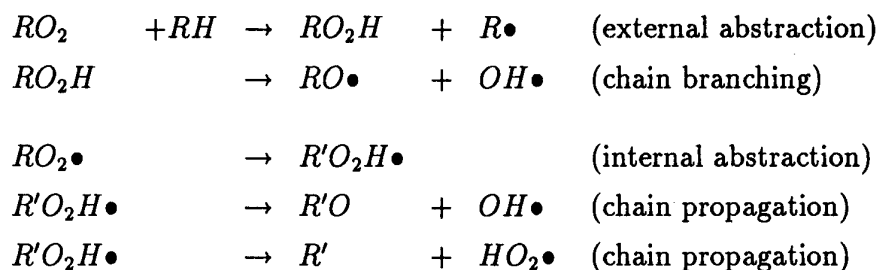
At medium temperature ($1100 \text{ K} > T > 900 \text{ K}$ at a pressure $P = 1 \text{ bar}$), additional chain branching behaviour is introduced by the following reaction sequence [12]:



At low temperature ($T < 900 \text{ K}$ at $P = 1 \text{ bar}$), there is so-called "degenerated chain-branching" [2,13], characterized by the fact that a main precursor of chain-branching (here: $RO_2 \cdot$ radicals) is decomposed at higher temperature ($T > 800 \text{ K}$), leading to an inverse temperature dependence of reaction rate (for n -heptane e. g. $R = C_7H_{15}$ isomers, $R' = C_7H_{14}$ isomers, $R'' = C_7H_{13}$ isomers; " \rightarrow " denotes irreversible reaction, " \leftrightarrow " reversible reaction):

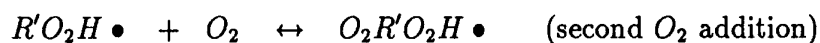


The $RO_2 \bullet$ radical formed can undergo external or internal H atom abstraction:

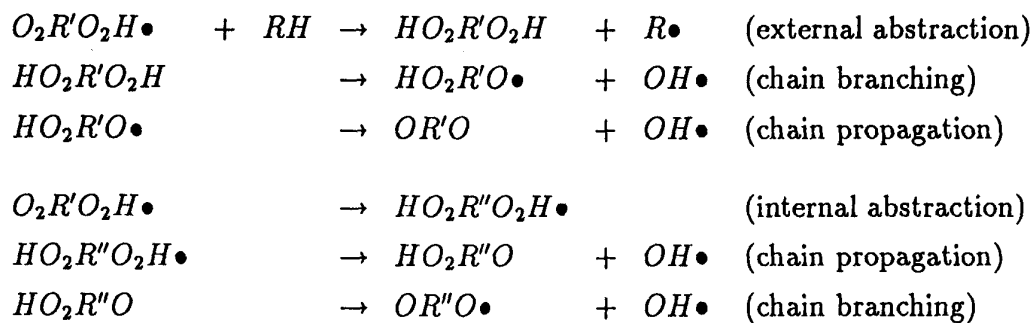


This means that external H atom abstraction leads to pronounced chain branching, whereas internal H atom abstraction (via ring formation) only leads to chain propagation.

All simulations at conditions of interest here show the internal H atom abstraction to be the reaction path preferred, if the rate coefficients taken from the literature are used (see [10,11] for further reference). Thus, no distinct acceleration of the ignition process can be expected as result of the first O_2 attack, as it is known from experiments of different groups [4-6]. As a consequence, the second attack of O_2 is considered in detail, as it is used e.g. in the simplified formal mechanisms describing low temperature ignition (see e.g. [7]):



Again, the $O_2R'O_2H\bullet$ radical formed can undergo external or internal H atom abstraction:



In contrary to the first O_2 attack, this means that both external H atom abstraction and internal H atom abstraction lead to chain propagation. Thus, a distinct acceleration of the ignition process should be expected as result of the second O_2 attack, explaining the experimental behaviour (see Fig. 1).

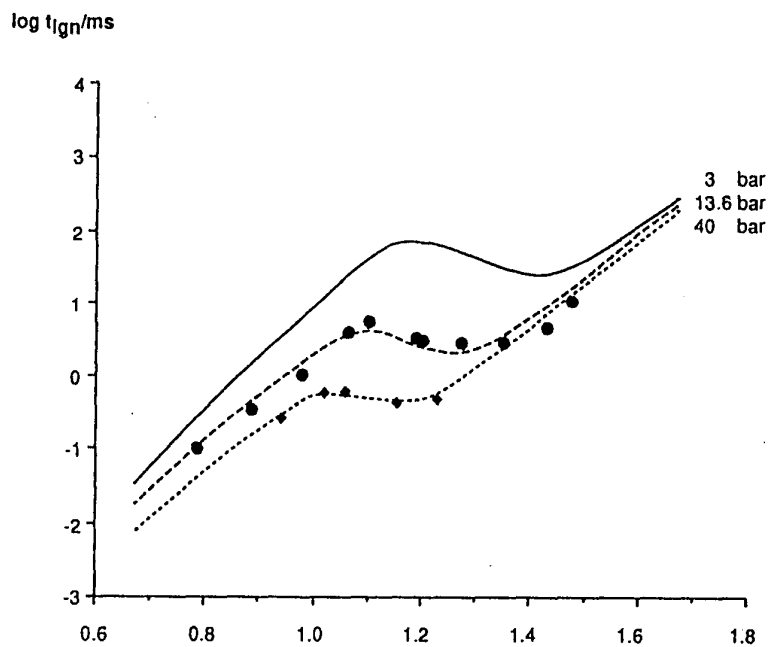


Fig. 1: Ignition times versus $1/T$ of stoichiometric n-heptane / air mixtures.
 Points: experiments (RWTH Aachen)
 Lines: calculations

2.2 Computation of Ignition Delay Times

Calculation of ignition delay times (or induction times) is performed by solving the conservation equations of the reaction system, considering the respective experimental conditions of pressure, volume, and temperature which, in some cases (e.g. end-gas of Otto engines), are time-dependent. Treating homogeneous mixtures, these equations represent then a system of ordinary differential equations with the time t as independent variable and with the species concentrations c_i as dependent variables. The equation system may be written as (see [12,14])

$$\dot{c}_i = \omega_i + c_i \cdot \left\{ \frac{\dot{p}}{p} - \frac{RT \cdot \sum \dot{\omega}_i}{p} - \frac{\dot{T}}{T} \right\} ; \quad i = 1, \dots, n$$

if the temperature T and the pressure p are given, or in the alternative formulation

$$\dot{c}_i = \omega_i - c_i \cdot \frac{\dot{V}}{V} ; \quad i = 1, \dots, n$$

if the temperature T and the volume V are given, with ω_i = molar rate of formation of species i , R = gas constant, n_S = number of species (typically 100–200 for large hydrocarbons); $c_i(t = t_0) = c_{i0}$ are the initial conditions. Due to stiffness of the equation systems considered, an implicit method is chosen for solution [15,16].

As an example, the computed dependence of ignition delay time from temperature is shown in Fig. 1 for a stoichiometric n -heptane/air mixture at $P = 13,6$ bar. Typical is the transition between high temperature and low temperature, taking place between 900K and 750K.

3. Assignments of Rate Coefficients

Despite the large number of species and of reactions expected in a chemical mechanism for ignition of the higher hydrocarbons, there is only a small quantity of reaction types, and therefore small quantity of rate coefficients.

At high temperatures, ignition occurs by molecular decomposition, near the center of its main chain, the rate expressions being only dependent on the type of C–C bond [10]:

$$\text{Secondary-secondary C-C bond: } k = 3.2 \cdot 10^{16} \exp(-81\,000 J/RT) s^{-1}$$

$$\text{Secondary-tertiary C-C bond: } k = 2.0 \cdot 10^{16} \exp(-78\,000 J/RT) s^{-1}$$

At lower temperature, initiation predominantly occurs by reactions between fuel and molecular oxygen with rates summarized in Table 1 [10].

	Primary	Secondary	Tertiary
<i>H</i> atom abstraction			
<i>RH</i> + <i>H</i>	$9.38 \cdot 10^6 T^2 \exp(-7700/RT)$	$4.5 \cdot 10^6 T^2 \exp(-5000/RT)$	$1.26 \cdot 10^{14} \exp(-7300/RT)$
<i>RH</i> + <i>O</i>	$1.67 \cdot 10^{13} \exp(-7850/RT)$	$1.3 \cdot 10^{13} \exp(-5200/RT)$	$1.00 \cdot 10^{13} \exp(-3280/RT)$
<i>RH</i> + <i>OH</i>	$1.43 \cdot 10^9 T^{1.05} \exp(-1810/RT)$	$6.5 \cdot 10^8 T^{1.25} \exp(-702/RT)$	$4.00 \cdot 10^{12} \exp(-443/RT)$
<i>RH</i> + <i>HO</i> ₂	$1.87 \cdot 10^{12} \exp(-19400/RT)$	$1.68 \cdot 10^{12} \exp(-17000/RT)$	$1.00 \cdot 10^{12} \exp(-14400/RT)$
<i>RH</i> + <i>CH</i> ₃	$6.5 \cdot 10^{11} \exp(-11600/RT)$	$6.10^{11} \exp(-9500/RT)$	$1.00 \cdot 10^{11} \exp(-7900/RT)$
<i>RH</i> + <i>CH</i> ₃ <i>O</i> ₂	$4.2 \cdot 10^{12} \exp(-20460/RT)$	$1.5 \cdot 10^{12} \exp(-17000/RT)$	$3.00 \cdot 10^{12} \exp(-15000/RT)$
<i>RH</i> + <i>O</i> ₂	$4.2 \cdot 10^{12} \exp(-49000/RT)$	$1.10^{13} \exp(-48000/RT)$	$2.00 \cdot 10^{12} \exp(-46000/RT)$
Alkyl radical isomerization			
(1, 4)	$1.10^{11} \exp(-21100/RT)$	$1.10^{11} \exp(-18100/RT)$	$1.00 \cdot 10^{11} \exp(-16100/RT)$
(1, 5)	$1.10^{11} \exp(-14100/RT)$	$1.10^{11} \exp(-11100/RT)$	—
(1, 6)	$1.10^{11} \exp(-21100/RT)$	$1.10^{11} \exp(-18100/RT)$	—
Alkylperoxy and hydroperoxyalkylperoxy radical isomerization			
(1, 4)	$1.10^{11} \exp(-20500/RT)$	$1.10^{11} \exp(-17000/RT)$	$1.00 \cdot 10^{11} \exp(-13500/RT)$
(1, 5)	$1.10^{11} \exp(-14600/RT)$	$1.10^{11} \exp(-11100/RT)$	—
(1, 6)	$1.10^{11} \exp(-15000/RT)$	$1.10^{11} \exp(-12000/RT)$	$1.00 \cdot 10^{11} \exp(-9000/RT)$
(1, 7)	$1.10^{11} \exp(-24000/RT)$	$1.10^{11} \exp(-20500/RT)$	—

Table 1: *H* atom abstraction reaction rates
Rates per equivalent *H* atom in cm³-mol⁻¹-sec units

Alkyl radicals produced by *H* atom abstraction from the fuel decompose at elevated temperatures through β -scission with a rate coefficient $k = 2.0 \cdot 10^{13} \exp(-28\,700 J/RT) \text{ s}^{-1}$ [10].

Isomerization of alkyl radicals via internal *H* atom abstraction is also given in Table 1.

At lower temperature ($T < 900 \text{ K}$), reactions of alkyl radicals involve addition of molecular oxygen. Following BENSON [13], the bimolecular rate coefficient of $2 \cdot 10^{12} \text{ cm}^3/\text{mol} \cdot \text{s}$ is taken. The reverse reaction rate coefficients recommended

by MORGAN ET AL. [17] of $2 \cdot 10^{15} \exp(-28\,000 J/RT)s^{-1}$ are used.

There are two major types of reactions of the RO_2 radical: The first is abstraction of H atoms from the major hydrocarbon species to produce alkyl hydroperoxydes ($ROOH$), which then decompose to produce $RO + OH$, followed by β -scission of RO . These sequences of reactions are of relatively minor importance for the higher hydrocarbons .

The most important step involves isomerization of the RO_2 radicals via internal H atom transfer, leading to a $R'OOH$ radical. The rate coefficient of this reaction depends on the size of the intermediate ring structure, on the type of H being abstracted, and on the number of equivalent H atoms [10]; see Table 1. The $R'OOH$ species then react mainly via a second addition of molecular oxygen, followed by another internal H atom abstraction. The same reaction rate coefficients as for the first ones are assumed. Following POLLARD [1], it is assumed that the first OH abstraction from $OOR''OOH$ leads to the formation of a carbonyl group, via internal rearrangement of the molecule with $k = 1.109 \exp(-7\,500 J/RT)s^{-1}$. The second OH abstraction, responsible for the chain branching, occurs with a higher activation energy: $k = 8.4 \cdot 10^{14} \exp(-43\,000/RT)s^{-1}$. The $OR''O$ radicals then decompose via β -scission.

The second possibility of consumption of $R'OOH$ is the decomposition into an alkene and HO_2 , which is of minor importance .

4. Automatic Generation of Reaction Mechanisms

4.1 Rule Oriented Programming

For the implementation, techniques from several areas of computer science were used, mainly from artificial intelligence (rule paradigm, tree structures) and computer algebra (canonical form technique). LISP is used as support system, as here the best flexibility regarding the data structures, the algorithm development and the user interface design is available.

In the artificial intelligence research several programming paradigms were developed, which facilitate the representation of complex knowledge contexts. As in the chemical reactions are an area with "exact" knowledge, which mostly

is encoded in rules written in natural language, the usage of the rule oriented program paradigm is most adequate.

The knowledge is formally coded in production rules of the following type:

$$\begin{array}{ll} Rn & \text{If } P_1 \text{ and } P_2 \text{ and } P_3 \text{ and } \dots \\ & \text{then } C_1 \text{ and } C_2 \text{ and } \dots \end{array}$$

The rule has a name (here "*Rn*") which later will be used for identification. A set of premises (here P_1, P_2, \dots) is linked by logical conjunctions (and, or, not); the premises are expressions testing the objects for certain properties. If all tests are positive, the conclusions (here C_1, C_2, \dots) are activated (the rule "fires"). E. g:

$$\begin{array}{ll} R2 & \text{If } (\text{is_alkane}(x)) \\ & \text{then } (\text{reaction: beta_scission}(x)) \end{array}$$

Most of the rules are formulated in a manner independent from each other; so it is possible to activate, deactivate, add and withdraw rules without recompilation.

At the moment the rules act on two semantic levels:

- On the production level reactions are deduced from new or generated species; a general inference machine activates each production rule for any relevant object or combination of objects exactly once.
- On a reformation level each new generated species is investigated for necessary reformations; here e.g. two neighboured radical positions are converted into a double bond.

In the course of the development a third level of rules was introduced, which plays a role of a meta rule: "rule Rx should be activated only if Ry did not yet fire". These meta rules define a unique sequence of dependency; they sometimes facilitate the description, but they create an additional dependency among the rules which reduces the flexibility.

4.2 Data Structures

It is most convenient to represent molecules as graphs, where the atoms are nodes and the molecular links are the edges. As complex analysis procedures are required, the sorted tree (ST) was selected among the different possible graph structures. A tree is a directed graph where one node plays the special role of a root. There are zero or more branches (links) from the root to the other parts of the tree, which then form sub-trees themselves. The branches are sorted lexicographically based on the atom weight: a branch b_1 is considered "heavier" as b_2 , if the first (leftmost) different atom in b_1 is heavier than in b_2 . Double or higher bounds are kept as labels of the links and they are integrated in the lexicographical ordering.

In order to get a completely unique representation, one selects among the different possible ST's of a molecule that one as "*canonically sorted tree*" (CST), which has an atom of the heaviest element class as root and which is the most important under the lexicographical ordering. The CST is canonical in the sense of computer algebra, as

- for a given molecule (ST) the corresponding CST can be computed by a straightforward (recursive) algorithm,
- two molecules are chemically equivalent if and only if their CST's are identical.

The CST is the most important means for the identification of generated molecules.

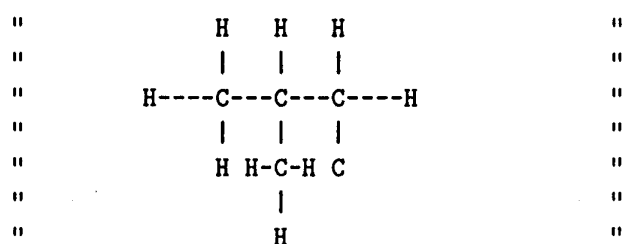
All molecules are represented as formally saturated; open bounds are saturated by an artificial "element" named \emptyset . This representation offers several advantages:

- The detection of radicals and radical points in a molecule is simple: look for an explicit \emptyset .
- The open bound can play the role of the root in a ST; that ability is used often as a radical point often is the origin of chemical activity.
- The formal correctness of a molecule can be simply verified by counting the links of a node and compare it with the valence of the atom; missing links so are not implicitly recorded as radicals.

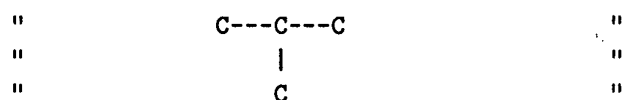
Practical considerations have led to a different handling of “missing” links: they are filled by *H* atoms automatically in most situations, as in the context of hydrocarbons this approach facilitates encoding of molecules.

4.3 2-Dimensional Structural Input

It is hard to generate tree structures by hand. Thus, a technique was developed which allows to “draw” molecules in two dimensions with ASCII characters, e.g.



or with the convention of omitted *H* atoms



4.4 Pattern Matching

In the rules for the automatic generation of combustion reaction systems the following types of tests in the premises are used:

- Classification of molecules by collecting and/or counting their atoms (e.g. *hydro-carbon*(*x*) ↔ *x* contains only *H* and *C*)
- Classification of molecules by looking for counting special branches (e.g. *has_branch_OOH*(*x*) ↔ *x* contains a *-O - O - H* group)
- Classification of very specific shapes of a parts of molecules.

While the first two types are coded as (enlargeable) set of test functions which operate directly on the ST of a molecule, the implementation of the third one

is much more complicated. Here a very general pattern matching technique is used. The local shape is described by a pattern, which is encoded as an ST like complete molecules. But here some of the branches can be variables. If now a molecule m is compared with a pattern p , first all ST variants of m with the same root as p are computed, giving m_1, m_2, \dots . In the next step each m_i is compared with p separately: constants (atoms, link labels) must match identically, while variables match anything. If there is no contradiction, the pattern fits and the variables are bound to the partial branches. These values now can be used to construct the reaction products.

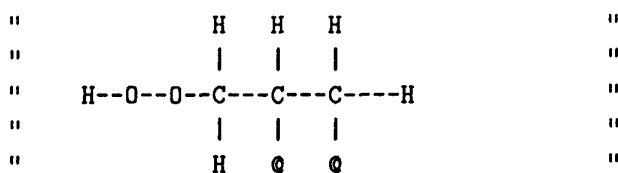
Example:

```
(mrule H1 (m)
  (prog (res)

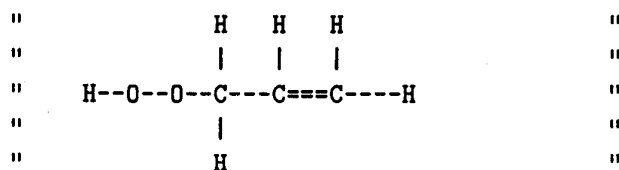
    (mpmatch ONCE m
      "          &1 &4          "
      "          | |          "
      "          @-----C---C-----@          "
      "          | |          "
      "          &2 &3          "

      (setq res (mpgen
        "          &1 &4          "
        "          | |          "
        "          C===C          "
        "          | |          "
        "          &2 &3          "
      )))
    (value res)
  ))
```

In this rule the first group of strings defines a pattern, which contains two adjacent C atoms, which both have an open link, and four variable links. This pattern e.g. fits for the molecule



where &1 is bound to the left part of the molecule, while all remaining variables are bound to a *H*. In the second part of the rule a new molecule is constructed from the components bound in the variables, which here results in



This is one of the rules on the reformation level.

There are several modes of pattern matching:

- ONCE:** only the first pattern fit is regarded,
- ALL:** all possible pattern fits are regarded and the rule body is executed for each fit separately.

A specific difficulty is the control of multiplicities. Here different formalisms were implemented for different question types, e.g. multiple matches are reduced, but their multiplicity is available as a number, or equivalent matches are counted explicitly. The last case is especially important, if reactions concerning *H* atoms are handled. Here one in general has multiplicities which enter the final rate calculation.

5. Results

Using the program and the reaction rate coefficients described above, it has been possible to generate a mechanism for calculation of ignition delay times of *n*-heptane/air mixtures. This mechanism contains at the moment 2400 reactions, and 620 different chemical species. Using an IBM 3090, one simulation lasts almost 20 minutes. The hand-written mechanism had 1000 reactions and 170 species, and calculation times were correspondingly shorter.

The results obtained are compared with the hand written mechanism and with experimental measurements in Fig. 2, for stoichiometric *n*-heptane/air mixtures, at $P = 13,6$ bar. The automatically generated mechanism also leads to the calculation of a negative temperature dependence between 900 K and 750 K.

Besides, a good agreement with the experimental measurements is shown on the whole range.

These promising results show that it will be possible to generate automatically mechanisms for oxidation of higher hydrocarbons.

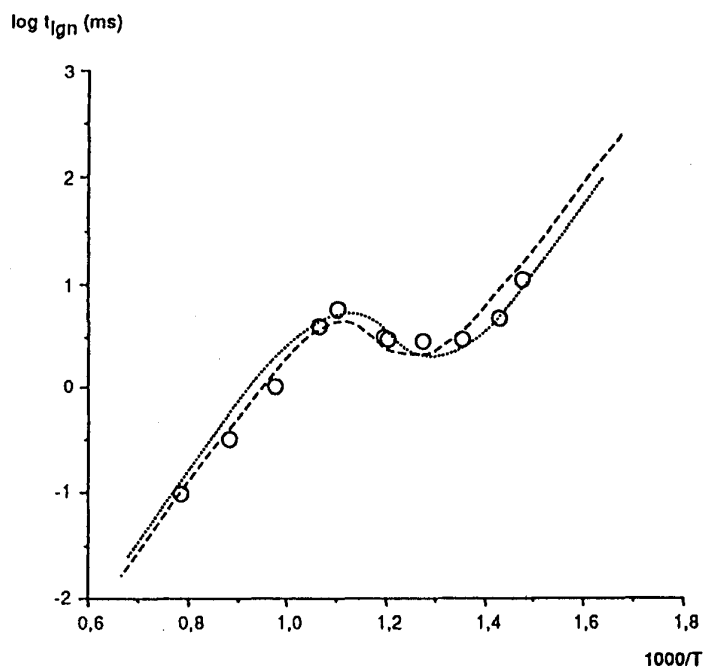


Fig. 2: Ignition time versus $1/T$ for a stoichiometric n-heptane / air mixture. $P = 13,6$ bar

- Measurements (RWTH Aachen)
- Simulations with automatically generated mechanism
- Simulations with hand-written mechanism.

6. Conclusions

Auto-ignition in hydrocarbon-air mixtures is complicated due to the large number of isomeric structures to be considered. However, there are only a few reaction types occurring so that reaction mechanisms can easily be generated automatically. In order to avoid generating mechanisms containing reactions and species not of any importance for the highest hydrocarbons, it will be necessary to limit the total number of species and of reactions, by giving new restricting rules. The rate equations resulting from this procedure can be subsequently integrated with modern numerical methods and the computers presently available. This automatic mechanism generation leads to the possibility to simulate quantitatively the auto-ignition behaviour of large hydrocarbons with air and thus to understand fundamental phenomena like two-stage ignition and negative temperature coefficients in combustion processes and to explain practical processes like e.g. Diesel engine ignition and Otto engine knock.

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