# MODELING VIRTUAL FUELS FOR HCCI-LIKE INTERNAL COMBUSTION ENGINES DEVELOPMENT

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## Abstract
Efficiency and cleanliness of internal combustion engines can be easily improved with better *after-design agents* like cleaner lubricants and fuels, tribo-coatings and innovative materials or complex exhaust after-treatment systems, but it is above all a matter of well-planned design from the beginning of engine development itself.
The rush for the *zero-emission vehicle* sets on the table the old chimaera of automotive engineers: the HCCI combustion engine. This particular engine has very high efficiency and produces neither PM nor NOx but, however, for its development, it cannot be simulated trustfully and completely with current virtual tools yet (because of the complexity of that kind of combustion) nor tested on real benches (because of the that kind of combustion is still hard to control).
Supported by *QuickSim©*, a Virtual Engine (VE) used in FKFS/IVK for series/motorsport/educational purposes, a better description of the combustion characteristics of gasoline surrogates has been developed by means of Virtual Reactors (VR), as far as flame speed and ignition point are concerned, and the results are presented in this work, as extract from the PhD final work of the author. [1]
This way, innovative combustions can be investigated and developed involving also unconventional fuels and following operations at real test benches where slight differences among traditional gasolines do affect tests results.

## Background
All possible strategies aimed to improve the efficiency of an engine would increase its specific power output and, above all, automatically lower its specific pollutant emissions. These strategies can involve friction and vibrations reduction, like less/lighter moving components and better lubrication, better *breathing* and higher compression ratios, faster combustions, particular scavenging timings, smart thermal managements, hybridization and so on. [2]
Nowadays, efficiency means cleanliness rather than performances and, besides the aforementioned technologies, innovative working cycles are arising, like those characterized by Low Temperature Combustion (LTC), which allows cleaner combustions, in a generic engine, in lean operation modes.

There are indeed particular engine designs, working with LTC principles, called Homogeneous Charge Compression Ignition (HCCI) [3], where a homogenous mixture – as in gasoline-like Spark Ignited cycles (SI) - is compressed and induced to auto-ignition – as in Diesel Compression Ignition cycle (CI).
In HCCI operating mode, as far as emission are concerned, the mixture is too lean to allow soot formation and the temperatures are not sufficiently high to produce nitrogen oxides. This way, emissions of the most harmful engine pollutants are limited (or avoided) at the root.

From a thermodynamics point of view, rapid homogenous combustions, lean mixtures and high compression ratios lead to very high overall efficiencies. [4]
However, working with HCCI cycles is not that easy, because a lean mixture is usually hotter than a rich one (no heat spent by unburned fuel vaporizing): to keep combustion temperature under control, the mixture has to be homogeneous in the whole chamber. Furthermore, the control of fuel auto-ignition and flame propagation are crucial to master these applications.

These last two properties, characteristic of a given fuel, are the reason of the absence of HCCI-like engines on the market, despite their clear advantages. In fact, the development of all those technologies aimed to control auto-ignition and flame propagation (or flame speed) pass thorough deep investigations and experimentation on engine proof stands but the effects of uncontrolled combustions may lead to tragic failures, with dramatic increase of development costs and efforts.
More than ever, VE gained a central role in HCCI-like engines development, exploring all possible design variations with no worries about expensive prototypes and rig damaging.

QuickSim©, a virtual engine developed in FKFS, is a well-known tool for internal combustion engines development, used since years for series, motorsport and educational purposes that is already been involved in successful research activities about HCCI combustion. [5]
Being HCCI combustion strongly fuel-dependent, the most important models in these kinds of simulations are those regarding flame speed, auto-ignition timings and thermodynamics properties of fuels. The next question about HCCI-like combustion is how gasoline/fuel recipe may help or hinder these applications.

The current set of fuel models equipping QuickSim© is not suitable to investigate unconventional fuels neither to discriminate among gasoline recipes differences so this would be a nice occasion to develop new and better gasoline surrogates with this software. This way, this VE could follow, and even predict, the real combustion behavior of different fuels even in HCCI modes, which may differ only for slight changes in their recipes, that can be noticed at the proof stand and discriminate if a test is successful or not.

## Modeling approach

Actually, QuickSim© uses a smart mechanism that may discretely trigger gasoline ignition [6]. A *generic* gasoline. For the Flame Speed description, QuickSim© uses a model proposed by Gülder in 1984, about a generic RON90 gasoline. [7]
To overcome these limitations, two VR has been set with CANTERA© in order to evaluate the behavior of gasoline surrogates ranging temperature, lambda, pressure and dilution (indicated as *cold EGR*). [8][9][10]
Auto-ignition VR is set as a 0-D constant volume bomb reactor. Flame Speed VR is a 1-D, grid-based reactor, which is of course time-dependent and requires way more calculation times then the other VR.

Selection of a suitable thermokinetics mechanism is as crucial as the design of the VE. The requirements are the following: a good set of mid-temperature reactions, a high number of low-temperature ones, the presence of all the chemical species which the surrogates are made of and, of course, a good balance between description and calculation times needed; the mechanism proposed by Fandakov (2017) has been chosen. [11]

## Auto-ignition

The recipe of a gasoline however, is more complicated than PRF/TRF surrogates (Primary Reference Fuel and Toluene Reference Fuel, respectively) and this limitation is evident more than ever in HCCI-like development where, at the real proof stand, light differences between several fuels can discriminate between successful tests or tragic failures.
These applications need new fuels virtual surrogates, capable of a better description than PRF/TRF but, after all, still simple enough to be evaluated by VR in acceptable calculation times.

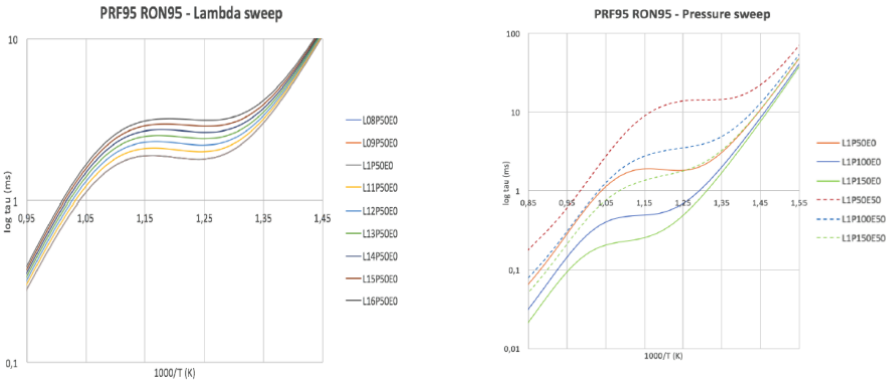


**Figure 1**. The effects of lambda and pressure sweeps on auto-ignition timings of PRF95. L is lambda, P is pressure (bar) and E is cold EGR (%). [1]

Comparing several recipes of real gasolines, six families of components have been recognized and, for each of them, their effects and main representatives have been screened until a new gasoline surrogate, made by six components, has been proposed and evaluated in the VR (see **Table 1**). In Figure 2 the behaviors of traditional surrogates, like PRF and TRF, and the new proposed surrogate, *MRF (Modeling Reference Fuel)*, are depicted. Of course, the *recipe* of MRF is closer than the others to the real fuel chosen as reference, despite all surrogates have the same RON 95 basis.

**Table 1.** Comparison between traditional RON surrogates (PRF), ultra-RON surrogates (TRF) and the proposed, more descriptive, six-components gasoline surrogate (MRF), suitable for unconventional combustion modeling. [1]

| | **PRF** | **TRF** | **MRF** |
|---|---|---|---|
| **Paraffines** | n-Heptane | n-Heptane | n-Heptane |
| **Isoparaffines** | iso-Octane | iso-Octane | iso-Octane |
| **Aromatics** | - | Toluene | Toluene |
| **Naphtenes** | - | - | cycle-Hexane |
| **Olefines** | - | - | iso-Octene |
| **Oxygenated** | - | - | Ethanol |

The Negative Temperature Coefficient (NTC) region is still present in MRF but less wide and, consequently, less decisive in affecting combustion control and behavior. In general, but particularly in HCCI applications, an accurate description of NTC phenomena is crucial in combustion control and the traditional fuel surrogates show NTC regions wider than they actually are, adding uncertainty to VE's control.

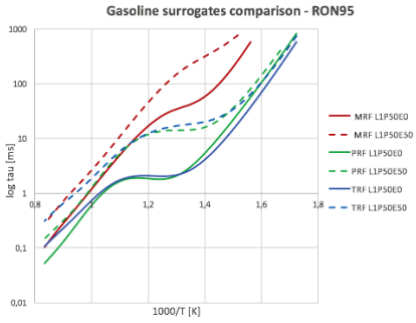


**Figure 2**. Comparison between auto-ignition profile of PRF, TRF and the new six-components gasoline surrogate MRF, all RON95 grade; with (dashed) and without (solid) cold EGR effect, cause of auto-ignition delay. L is lambda, P is pressure (bar) and E is cold EGR (%) [1]

## Flame speed

Comparing CANTERA©'s VR and old Gülder's flame speeds, it seems that Gülder offers higher peak values (see Figure 3); this is not acceptable in HCCI investigations since high flame speeds could be source of misinterpretations in QuickSim© and lead to inexistent knocking and detonation phenomena. Moreover, Gülder is not able to calculate the flame speed when EGR is over about 40%, limiting the opportunities of investigation. The flame speed by Gülder is not suitable for HCCI unconventional combustions. In turn, the VR approach offers lower peak temperatures, the possibility to range operating conditions to support VE operations, the capability to blend gasolines with ethanol and water, and it well fits the initial request from QuickSim© for a fast, reliable and flexible flame speed model.

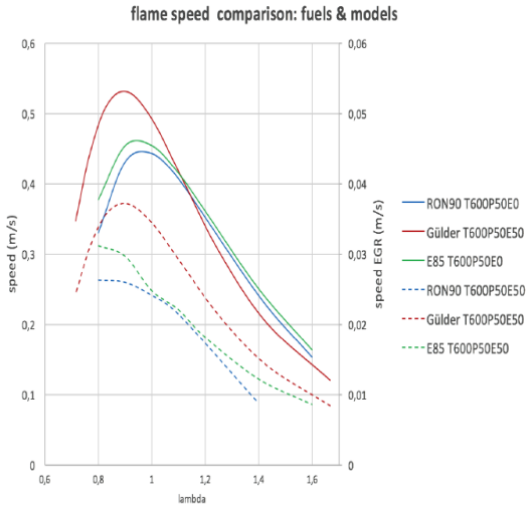


**Figure 3.** Differences of flame speed between TRF40, E85-TRF40 and Gülder RON90 gasoline. Of course, TRF40 is as knocking resistant as PRF90. L is lambda, P is pressure (bar) and E is cold EGR (%). [1]

## Outlook

Two virtual reactors for auto-ignition (0D) and flame speed (1D), coupled with a smart thermokinetics mechanism, have been set with CANTERA©, allowing the development of a new six-components gasoline surrogate, able in turn to retrace real fuels more precisely than traditional three components surrogates, like PRF and TRF. Data collecting in 4-D look-up tables and VE implementation is still on going, but the study about HCCI combustion (and even the ideal HCCI fuel) has already led to encouraging results, achieving engine settings for a regular and controlled HCCI combustion at the test bench. Yet, using a commercial gasoline. Ethanol blends and pure ethanol are meant to be tested as soon as the VE is finally ready to fully use these new fuels descriptions [1].

**Nomenclature**

| | |
|---|---|
| *CI* | Compression Ignition |
| *FKFS* | Forschungsinstitut für Kraftfahrwesen und Fahrzeugmotoren Stuttgart |
| *HCCI* | Homogeneous Charge Compression Ignition |
| *LTC* | Low Temperature Combustion |
| *MRF* | Modeling Reference Fuel |
| *NOx* | Nitrogen Oxides |
| *NTC* | Negative Temperature Coefficient |
| *PM* | Particulate Matter |
| *PRF* | Primary Reference Fuel |
| *SI* | Spark Ignition |
| *TRF* | Toluene Reference Fuel |
| *VE* | Virtual Engine |
| *VR* | Virtual Reactor |

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