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### Contents

# *Degree Centrality of Combustion Reaction Networks for analyzing and modeling combustion processes*

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## Abstract

Combustion research still needs more advanced fundamental understanding of combustion chemistry and dynamics from molecule scale to particle. The latter is also needed for soot and nanoparticles formation and combustion system control such as Homogeneous Charge Compression Ignition (HCCI) engine, and flame regimes and instability. The complex interactions between hundreds of species linked within thousands of reactions continue to be a challenge to analyze and model. The focus of this paper is to develop a method to facilitate the modeling and analyzing of the detailed kinetics chemistry of fuels combustion. Through the use of Combustion Reaction Networks (CRN) analysis of degree centrality, principal species are identified during a combustion process by exploiting the introduced definition of principal species. A principal, central or the more active species of a combustion process, at a specific time step or cell of area/volume mesh, is the more tied up to other species in the CRN and so have the largest value of degree centrality. The accuracy of the dynamic identification of principal species, locally adapted to the thermochemical conditions at each time step/cell of the simulated combustion process, used by the employed Directed Relation Graphs (DRG) method of mechanisms reduction, is proved. The simulations were carried out using an adjusted Dynamic Adaptive Chemistry (DAC) approach of detailed chemistry implementing. It is demonstrated that an ‘active’ species in a combustion system would not necessary be considered as a part of important species set needed for its predictive simulations.

**Key words:** Combustion Simulation, Network Analysis, Dynamic Adaptive Chemistry, Directed Relation Graph, Mechanism Reduction.

## 1. Introduction

Chemical reaction networks are widespread in many fields, for example cellular biochemistry [1, 2], genetics [3], nomenclature of constitutional or steric isomers, valence isomers [4], catalytic reaction mechanisms [5] and molecular dynamics simulation data of bulk water studies [6]. Generally, methods for analysis of network systems are widely-sought and there is high need for their development [7, 8]. Network structures could be analyzed via graph-theoretic methods [9] or methods which focus on systematic network decomposition or metabolic pathway analysis [10].

The ideas of Graph-theoretic methods were initiated by Leonhard Euler in 1730, studying the problem of the Seven Bridges of Köningsberg [11]. Graph theory is the study of graphs, which are mathematical representations used to model the relationships among objects. A graph is made up of vertices, nodes, or points which are connected by edges, arcs, or lines. At present, graph theory is used as a modeling and analyzing tool for many practical problems of biochemistry [12], electrical engineering [13], computer science [14] and human life [15]. A general overview on graph theory could be found in Harary’s Graph Theory [16] and Berge’s Graphs and Hypergraphs [17].

A predictive simulation of engines and flames performance and emissions requires the implementation of validated detailed kinetic chemistry for a wide operating conditions into a Computational Fluid Dynamics (CFD) code. This requirement leads to a significant increase of computation time to solve the nonlinear stiff ordinary differential equations (ODEs) for each CFD computational cell. The common approach to solve these challenges for specific operating conditions is to build an enough small reduced mechanism which will be used in larger scale simulations after trying to accumulate in the maximum information from the detailed one by different optimization methods [18-20].

The numerical simulation of reactive flow using CFD codes requires the solution of a set of stiff ODEs of conservation of mass, momentum, energy and chemical species. The simulation of auto-ignition delay time of the adiabatic, constant volume and closed reactive system can be governed by the following two equations of energy and chemical species conservation:

$$\rho \frac{dy_k}{dt} = \dot{\omega}_k W_k \; ; k = 1, 2, \dots, K$$

$$\rho c_v \frac{dT}{dt} = - \sum_{k=1}^{K} \dot{\omega}_k W_k u_k$$

where $T$, $c_v$, $\rho$, $y_k$, $W_k$, $u_\mathrm{k}$, $\omega_k$, and $K$ denote temperature, constant-volume specific heat capacity and density of gas mixture, species mass fraction and molecular weight, internal energy and production rate of the $k^{\mathrm{th}}$ species, and species number, respectively.

The predictive combustion simulations incorporate essentially detailed chemical mechanisms into CFD calculations. The using of detailed chemistry produces a large number of stiff ODEs to solve within the CFD framework, and thus results in exceedingly long CPU times. The reduction of mechanisms at specified operating conditions of temperature, pressure and species concentrations allows the elimination of species and corresponding reactions that have a negligible effect on the rate of heat release and on the rates of target species production. As a result, the set of ODEs becomes smaller and then faster to solve. However, the use of a reduced mechanism in calculation codes might generate lower accuracy of the predicted results compared to that obtained using the full mechanism. Therefore, the Dynamic Adaptive Chemistry (DAC) approach, proposed by Liang et al. [21], could be the most useful adopted strategy for the purposes of CFD calculation, accuracy and low CPU time. Several studies have explored the application of this technique [21-27] which is applied locally, at each time steps/cells, using accurate (validated) reduced for the local thermochemical conditions. There are two ways to apply this strategy, the first employs the on-the-fly generation and then the immediate implementation of reduced mechanisms at each time step or cell [21-24] of combustion simulation and the second way is to generate a tabulated archive library of reduced mechanisms and classifying them depending on the different ranges of operating conditions [25, 26] to be implemented farther by the DAC approach.

Numerical solutions encountered in flames and engines for a wide range of thermochemical conditions needs the employment of algorithms, such as in situ Adaptive Tabulation (ISAT) [25, 26] or operator splitting schemes [27], to manage the integrated solving of ODEs system governing the reactive flows and the stiff nonlinear ODEs system governing the chemical reactions to achieve calculation convergence with lower CPU time cost.

The generation of reduced mechanisms on-the fly especially at each time step/cell requires fast and efficient reduction methods, in term of large degree of selective reduction in species and reactions, to achieve the purposes of getting less simulation time and more adapted generated reduced mechanisms compared to those using the detailed one. For these objectives, the DRG reduction method was adopted based on the removal of less-important species and their related reactions using the search algorithm of Lu and Law [28] which will be presented in more details in paragraph 2.1. DRG approach for mechanisms reduction requires the definition of principal/target species set which can simply consist of the fuel, oxidizer and important radicals [28]. If accuracy is required for additional phenomena such as NOx predictions, soot precursors/nanoparticles nucleus, a corresponding species (i.e. NO, acetylene, $SiO_2$ or/and ….) should also be included in the target set. The use of such set of principal species will scale up the reduction time of detailed mechanism. Therefore, the proposed coupling of the DRG reduction method with a characteristic network analysis parameter, discussed in paragraph 2.2, allows the dynamic selection, at each time step/cell, of one principal species validated for the specific thermochemical condition of simulation.

In fact, more efficient DRG methods with relatively higher reduction time have been developed such as the error propagation method (DRGEP) [21, 29-31]which permits to show the influence of the accumulated and propagated errors by the elimination of the less-important species set on the target one (i.e. NOx, soot precursors or nanoparticles nucleus), and the DRG method with sensitivity analysis (DRGASA) generating higher accurate reduced mechanisms but also with more computational time needed for the sensitivity analysis [32].

The performance of the DAC application, CPU time cost and simulation errors compared to the use of ordinary detailed chemistry, is influenced by the employed reduction technique and the thresholds of the reduction level. The impact of reduction methods and their thresholds on simulation errors of DAC application have been studied by:

- Gou et al. [33] using a reduction method of Path Flux Analysis (PFA) for auto-ignition simulations.
- Oluwole et al. [34] using Decoupled Species and Reaction Reduction (DSRR) and DRG approaches for auto-ignition and laminar flame simulations.
- Xie et al. [35] obtained lower relative errors by using Time-Scale and Jacobian-aided Rate Analysis (TSRA) reduction method rather than that of using DRG technique by an on-the-fly application of DAC for the simulation of auto-ignition and laminar flame process.
- Ren et al. [26] have studied the effect of DRG reduction threshold on the errors of temperature and species concentrations prediction of turbulent methane/air flames simulations using the DAC implementing approach.
- Zhao et al. [36] employed the Betweenness Centrality (BC) of chemical network analysis to generate skeletal mechanism for a given pressure, temperature and species concentrations. BC measured the relative connectivity of a source of species, Fuel, $O_2$, …, to a target species, $CO_2$, NO, …, in a network, and thus is based on the shortest paths passed by other species between the

larger BC values are the shortest paths connecting the source and target nodes, are incorporated in the skeletal mechanism from high to low levels. The built skeletal mechanisms using BC chemical network analysis predicts generally auto-ignition phenomena better than that of using the DRG approach.

The aim of this work is to present a qualitative analysis of chemical reaction networks, of degree of centrality in order to identify the principal species, at each time step/cell, of a combustion process simulation. The latter is useful to improve the accuracy and the fast calculations of the more appropriate and enough small reduced mechanisms generated by the employed DRG method of reduction. The on-the fly implementing of these reduced mechanisms has been effectuated using an adapted DAC.

The numerical simulations have been achieved using CANTERA software package [37] and the GRI-3 detailed mechanism of G.P. Smith et al. [38] for the studies of $C_1$-$C_3$ alkanes. The combustion simulations of $n$-heptane have been done using the $n$-heptane mechanism from LLNL[39].

## 2. Approaches and applications

### 2.1. Directed Relation Graphs

The DRG basic method of removal of unimportant species and reactions from a detailed mechanism of ethylene oxidation has been adopted by Lu and Law [28]. The following short presentation linked to graph theory could be a preferred step to introduce the employed reduction technique and the adopted building strategy of Combustion Reaction Networks (CRN). The importance of a species in a mechanism can be determined from the influence of its removal impact on the prediction of a principal species or of a set of principal species. In the graph theory, each point (vertex) of a CRN representation represents a species, and in the DRG method, the existing of an edge from $A$ to $B$ ($A \rightarrow B$) means that if and only if the elimination of species $B$ may directly induce significant error in the production rate $R_A$ of species $A$. The paper of Lu and Law [28] offers the detailed mathematical equations that describe the

DRG method. The definition of the coefficient $r_{AB}$ quantifies the normalized contribution of species $B$ for the production rate of a principal species $A$ in a chemical mechanism consisting of $n$ reactions:

$$r_{AB} = \frac{\sum_{i=1}^{n} |v_{A,i} w_i \delta_{Bi}|}{\sum_{i=1}^{n} |v_{A,i} w_i|},$$

where $w_i$ represents the net rate of $i$ th reaction, $\nu_{A,i}$ is the stoichiometric coefficient of species $A$ in this $i$ th reaction and $\delta_{Bi}$ takes the value 1 if the $i$ th elementary reaction involves species $B$ and takes the value 0 if it's not.

As a result of this work, the selection of the principal species $A$ will influence the performance of the DRG reduction method to build predictive reduced mechanisms by the selective elimination from the detailed one the less important species, $k$, and their related reactions, in which $r_{Ak} < \varepsilon$, where $\varepsilon$ is a specified fixed threshold (< 1). No specific rule to define the DRG reduction threshold, where the effects of this threshold on the predicted results errors can be a studies subject as done by Ren et al. [26].

The DRG reduction approach adopted in this study requires the selection of a principal species for the generation of reduced mechanisms. As the use of a principal species set requires more computational time, depending on the number of principal species, to reduce the original mechanism, and the quality of the generated reduced mechanisms depends on the selected principal species. Therefore, a dynamic selection of locally adapted principal species, follows the local thermochemical conditions at each time step/cell of the simulation, will be proposed by exploring the CRN analysis of degree centrality.

## 2.2. Chemical Reaction Network

A Chemical Reaction Network (CRN) can be represented by a dynamic system of reactional scheme that changes within time. In a chemical reaction scheme, with $K$ reacting species and $n$ reactions, reactions could be represented by the form:

$$\sum^{K} v'_{ij} X_i \rightarrow \sum^{K} v''_{ij} X_{i,} \quad j = 1,2,\ldots,n$$

where $X_i$ are the chemical species names participating in the full reaction scheme. The coefficients $v'_{ij}$ and $v''_{ij}$ represent the number of species molecules $X_i$, stoichiometric number, participating in the $j$-th reaction for reactant and product stages, respectively.

The dynamic changes with time step/cell, and the complexity of the resulted CRN graph couldn't be explored fully without oriented analyzing tools. For this purpose, Aric et al. [40] offered a wide documented Python language software package for the creation, manipulation and studying of such dynamic and complex network structures that has been partially used for the building and the analyses of the studied CRNs in this work. Using the definition of the rate coefficient $r_{AB}$, presented in paragraph 2.1., a CRN can be then built automatically by applying the $r_{ij}$ as a connection weight from species $i$ to species $j$, where $i$ and $j$ cover all the mechanism species, one by one, and using the condition $r_{ij} < \varepsilon$ to ignore the lower weighted edges from the built CRN. Figure 1 shows part of a complex CRN graph generated automatically for a methane ignition process, under the conditions of temperature $T$= 1500 K, Pressure $p$= 1 bar, and equivalence ratio $\phi$= 1. This CRN graph, figure 1, represents a map of the most effective production contribution of all the mechanism species for every species in the mechanism and at a specific thermochemical condition, $t$= 1 ms.

It's important to notice that the global network analysis, used in this work, uses a macro perspective to study the physio-chemical properties of a CRN structure. This study focuses on the global network analysis tools that support the employed DRG reduction and DAC implementing approaches.

The degree ($k$) of a node, a specific species, describes the number of edges linked to this node/species and so it indicates the contribution weights of other species to produce/consume this species, hence, the average degree of a network will present the average of degrees over all nodes in the network [11, 16].

The degree centrality, in graph-theoretical terminology, defines the number of edges adjacent to a specific node [41]. The simplest explanation of actor/species centrality is that the central actors must be the most active because they have the most ties to other actors in the network or graph [42]. As in the introduced building approach of CRN, an edge linked to any two species in the network characterized the production or the consumption contribution of one of these two species to the other; then the degree centrality analysis permitted the estimation of the activity, number of ties, of an actor ‘species’ in the studied CRN. Therefore, the centrality degree of a species, species activity, can be defined as the number of links that contribute to the production/consumption of a selected species by other species in the built CRN at specific thermochemical conditions of time step/cell of a combustion process simulation. The latter initiates the following species activity analysis during the auto-ignition of methane/air fueled a Rapid Compression Machine (RCM) at conditions of $T$= 1500 K, $p$= 1 bar and $\phi$= 0.25 and 2.

Figures 2 and 3 present the timing history of temperature and normalized degree centrality (NDC) for stable species and representative radicals of low-intermediate and high temperature chemistries, respectively, of methane/air fueled RCM at combustion conditions of $T$= 1500 K, $p$= 1 bar, $\phi$= 0.25 and 2. Figure 2a shows that the degree of centrality (activity) of oxygen is more important than that of methane and so is that of hydrogen compared to formaldehyde, figure 2b, for the two studied equivalence ratios and the whole duration. It could be observed from figure 3a that at low and intermediate temperatures, the selected radicals $CH_3$ and $HO_2$ have distinguished values of degree centrality for also the two studied equivalence ratios and the whole duration. The activity of hydroperoxy radical is higher than that of methyl radical at all the time steps and for the two different equivalence ratios (lean and rich conditions). It can be also observed that there is a decrease in the activity of methyl and hydroperoxy radicals after the ignition stage where the high temperature chemistry of H, O and OH radicals takes place. The activity values of the selected reactants, H and OH in figure 3b, take generally higher values for H than OH. These two radicals show more activity at lean condition $\phi$= 0.25, especially during the pre-ignition stage, compared to that at rich condition $\phi$= 2. An oscillated behavior of the degree of centrality was observed for the studied species during the pre-ignition stage, and this indicates their unstable activity level before the auto-ignition phase, and thus is related to the persistent variation of system thermochemical conditions of low, intermediate to high temperature chemistries. It could be noticed also that the activity of the high temperature chemistry radicals is more important than that of the low-intermediate temperature chemistry radicals for the studied conditions.

Figures 2 and 3 showed the dynamic change in values of the degree centrality of some main species and so the variation of their activity order as a function of time for the studied RCM combustion conditions. This quantity, degree centrality order of a CRN, is used then to introduce a definition of principal species. A principal species of a combustion process chemistry at a specific time step/cell is the more active one; has the higher value of degree of centrality.

### 2.3. Dynamic Adaptive Chemistry

The principal of the Dynamic Adaptive Chemistry (DAC) method is illustrated in figure 4 which is captured for methane/air oxidation in a RCM at $T$= 1500 K, $p$= 1 bar and $\phi$=1, figure 4a, Homogeneous Charge Compression Ignition (HCCI) engine where $T$= 1500 K, $p$= 1 bar, engine speed= 600 rpm, compression ratio=17 and $\phi$= 1, figure 4b, and laminar premixed flame where $T$= 300 K, $p$= 1 bar and $\phi$= 1, figure 4c. The evolution of the relative number of important species (RNIS) requested to be conserved in reduced mechanisms compared to that of detailed one as a function of time, crank angle or height above the burner (HAB) is presented. This RNIS depends on the selection threshold $\varepsilon$ presented in paragraph 2.1 and on the thermochemical conditions of time step/cell of the simulated combustion process. When RNIS takes the value of 1, this means that the DAC method must implement the full detailed mechanism. It can be also observed that at the ignition stage, figures 4a-b, and flame zone, figure 4c, where the low-intermediate and high temperature chemistries are all important for the combustion process, the number of species to be conserved in reduced mechanisms is the highest one.

Figures 5a-b show two examples of the influence of initial mixture temperature, $T$= 700, 1000 and 1300 K for $\phi$= 1, and equivalence ratio, $\phi$= 0.25, 1 and 2 for $T$= 1000 K, on the temperature history of the RNIS for *n*-heptane/air mixture fueled RCM combustion conditions at $p$= 1 bar, respectively. It can be observed that the RNIS incorporated in the local reduced mechanisms increases with the increase of the inlet mixture temperature from 700 to 1000 or to 1300 K at $p$= 1 bar especially for the prediction of pre-ignition and ignition stages. This result corroborates the merging requirement between the high and the low-intermediate temperature chemistries for the accurate simulation of these two stages. Figure 5b shows also similar behavior in the pre-ignition and ignition stages of *n*-heptane auto-ignition, which indicates nearby incorporating of chemistries during these two stages for the three studied equivalence ratios at $T$= 1000 K and $p$= 1. Above 1000 K, where the high temperature chemistry becomes important, the RNIS increases with the equivalence ratio including more important species for the accurate prediction of richer conditions. It can be also concluded from figures 4 and 5 that the most principal variations of the RNIS used in reduced mechanisms take place during the pre-ignition and ignition stages for the engine cases or in preheat and reactive zones for the case of 1-D laminar premixed flame, where occurs the main progress of low-intermediate and high temperature chemistries of the studied combustion processes.

The DAC approach of the on-the-fly mechanism implementing in CFD codes [21-24] is the most accurate by the use of reduced mechanisms which are validated for the local thermochemical conditions. On the other hand, it’s expensive in CPU time because of the full mechanism reduction at each time step or cell. Therefore, the DAC implementing strategy presented in figures 6 and 7 is proposed in this work to get the most suitable performance in terms of accuracy and fast calculation. The lack of an implicit thermochemical condition to order an automatic implementing need of a new reduced mechanism by the DAC is covered for the studied auto-ignition phenomena by a time condition presented in figure 6. Figure 6 describes the application diagram of the proposed DAC implementing approach. The timing key condition orders the generation/implementing execution of a new reduced mechanism regarding the new local thermochemical conditions at the beginning of each predetermined time ranges, $N_t$, of the studied ignition delay time. The pre-estimation of ignition delay time attends using empirical equations [43]. Figure 7 presents an example of the variation of the RNIS as a function of time using the proposed DAC implementing approach where $\varepsilon$=1.10$^{-7}$ and $N_t$= 7, for methane fueled a RCM at conditions of $T$= 1500 K, $p$= 1 bar and $\phi$=1. The simulations start always with the full mechanism that will be reduced at the beginning for the initial operating conditions, and then reduced again for the new local thermochemical conditions of the time step located at the beginning of each predetermined time ranges, $N_t$. The effects of the prefixed time ranges on the predicted results errors will be a discussion subject in paragraph 3.

Generally, the proposed DAC implementing approach consists of generating previously/on-the-fly of locally adapted reduced mechanisms and then its implementing for each prefixed range of time steps or area/volume of mesh cells. This preselected range of time steps or area/volume of mesh cells becomes a performance criterion of the approach.

## 3. Discussion

The definition of principal species is validated by coupling the proposed DAC implementing approach and the DRG reduction technique, and comparing the predicted results using two selection methods of principal species for the DRG technique application. A static method, applying fixed predefined selection of principal species for all the simulation time, such as Fuel, $O_2$, … or other intermediate species like H, $HO_2$, …, and a dynamic method of principal species selection, applying a variable principal species in function of calculation time by exploiting the definition of principle species introduced in paragraph 2.2. Practically, the principal specie is that has the highest degree centrality of the CRN species at the specific time step/cell of calculation.

Figures 8a-b present the variations of relative error *Rer* percentage, obtained between the predicted results using the ordinary simulation with full mechanism and that of the DRG-DAC application conditions of $\varepsilon = 1.10^{-7}$ and $N_t = 11$, as a function of dynamic (Dyn) and fixed predetermined principal species selection such as $CH_4$, $CH_3$ or H, for the simulations of methane fueled a RCM at combustion conditions of $T = 1500$ K, $p = 1$ bar and $\phi = 0.25$ and 2, respectively. The relative error is calculated for the predicted timing history, $n_t$ values, of temperature and some main species concentration, $X_t$, using the following equation:

$$Rer = \sum_{i=1}^{n_t} \left| \frac{X_i(full\ mechanism) - X_i(with\ DAC + DRG)}{X_i(full\ mechanism)} \right| / n_t$$

It can be observed from figure 8 that the adopting of dynamic selection strategy of principal species using the CRN analysis of degree centrality gives generally more accurate results comparing to that using a static principal species selection for the DRG reduction technique. The employment of static principal species can generate high relative errors as the studied cases of $\phi = 0.25$, figure 8a, using the fuel or methyl radical as principal species. The observation discussed in paragraph 2.2 that hydrogen atom has generally the highest values of degree centrality during the overall simulation time of studied ignition cases, agrees completely with the comparatively low relative error percentage presented in figure 8, using this radical as static principal species and comparing to that of using the dynamic selection method of principal species, where the hydrogen radical is dominated as principal species at the most of the time steps of simulation.

Figure 9 shows an influence of equivalence ratio on the average, sum of RNIS at each time step divided by the number of time steps, of the employed RNIS in the generated reduced mechanisms. The variations are presented in function of dynamic (Dyn) and static (i.e. H, $CH_3$ or $CH_4$) selection of principal species used by of the DRG-DAC application conditions of $\varepsilon = 1.10^{-7}$ and $N_t = 11$. The simulations are effectuated for the two equivalence ratio of 0.25 and 2 of methane fueled a RCM at conditions of $T = 1500$ K, $p = 1$ bar. These results indicate that it is evident to generate relatively high relative errors by such selection of static principal species (i.e. $CH_3$ and $CH_4$) but with low RNIS average, so lower cost of CPU time. Noting also that the needed RNIS averages for the rich condition simulation of $\phi = 2$ are higher than that for the studied lean condition of $\phi = 0.25$ as seen and discussed before for figure 5b.

The influence of number of time ranges on the performance of the DRG-DAC application conditions of $\varepsilon = 1.10^{-7}$ and dynamic selection of principal species is presented in figure 10. It shows the variation of relative error percentage as a function of time ranges number of the predicted values time history of temperature and some selected species concentration of $CH_4$, $C_2H_2$, CO and $H_2$, for methane fueled a RCM at conditions of $T = 1500$ K, $p = 1$ bar and $\phi = 0.25$ and 2, figures 10a and b, respectively. For the two studied equivalence ratios, rising the number of time ranges produces more accurate predicted results, comparing to that of full mechanism, which responses to the DAC implementing of more appropriated reduced mechanisms to the local thermochemical conditions. The influence of time ranges number of the rich condition simulations of $\phi = 2$ is obviously higher than that for the studied lean condition of $\phi = 0.25$, indicating the need of more adapted reduced mechanisms to thermochemical conditions for the accurate prediction of rich conditions combustion. The adopting of time ranges number $N_t = 11$ for the simulations of the two equivalence ratios presented in figures 8 and 9 is then well justified. The user has to balance between the most suitable performance in terms of accuracy and fast calculation for a specific combustion modeling by his choice of the reduction threshold and the ranges of time steps or area/volume of mesh cells for the DAC implementing.

The indexing order of species activity, decreased values order of degree centrality of CRN species at specific simulation time, is tested as a reduction method to generate skeletal mechanisms incorporating a prefixed number of the more active/higher degree centrality of species in the studied CRN and their associated reactions. The application of this reduction approach showed the need of relatively higher number of species to be preserved in the generated reduced mechanisms for producing similar predictive results comparing to that using the DRG technique of reduction. Therefore, it could be concluded that a principal species is not necessary an important species to be preserved in reduced mechanisms, and the invers that an important species for the accurate prediction of a combustion process simulation is not necessary to be a principle species at fixed thermochemical conditions of time/cell. As Cantera utilizes object-oriented concepts and the users can explore the different phase models with limited changes to their overall code [37], an estimation of simulations real CPU times to be usefully compared was unfortunately not available.

## 4. Conclusion

Real complex networks such as combustion reaction networks, require analyzing methods which can examine systems that have parameter-uncertainty, high dimensional state space and non-linear terms. Degree of centrality analyzing method, which connects a combustion reaction network structures to its dynamic systems, was demonstrated not only for its simplicity but also for its advantageous. Such types of specific analysis might drive better understanding of particular combustion processes behaviors and more improvement to their modeling performance.

The focus of this work was to:

- Develop and extend some gainful of networks analysis methods in order to understand and analyze better the behavior of kinetic mechanisms which drive this complex physio-chemical phenomenon of combustion.
- Enhance the simulations performance of combustion processes by using the DAC implementation and the DRG reduction approaches coupled with a specific CRN analysis parameter of degree of centrality.

A definition of principal/active species during combustion processes simulations was introduced and validated successfully. A principal species has the highest value of degree of centrality at a specific time step/cell of simulations. The dynamic identification and implementing of locally adapted principal species to thermochemical conditions permitted the performance improving of combustion simulations, fast and accurate.

The unsuccessful testing of the ranking order of principal species identified by the degree of centrality analysis as a reduction technique of detailed chemistry can lead to the conclusion that ‘active’ species do not necessary belong to the important species set which are required for predictive combustion processes simulations.

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# Figures

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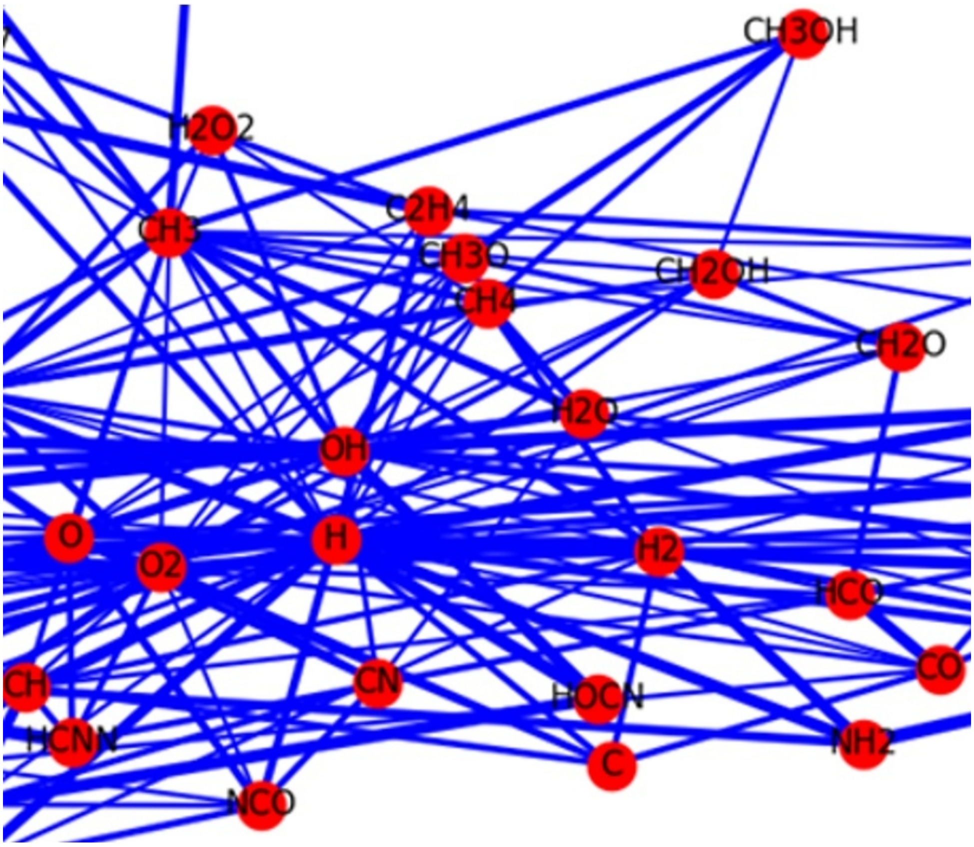
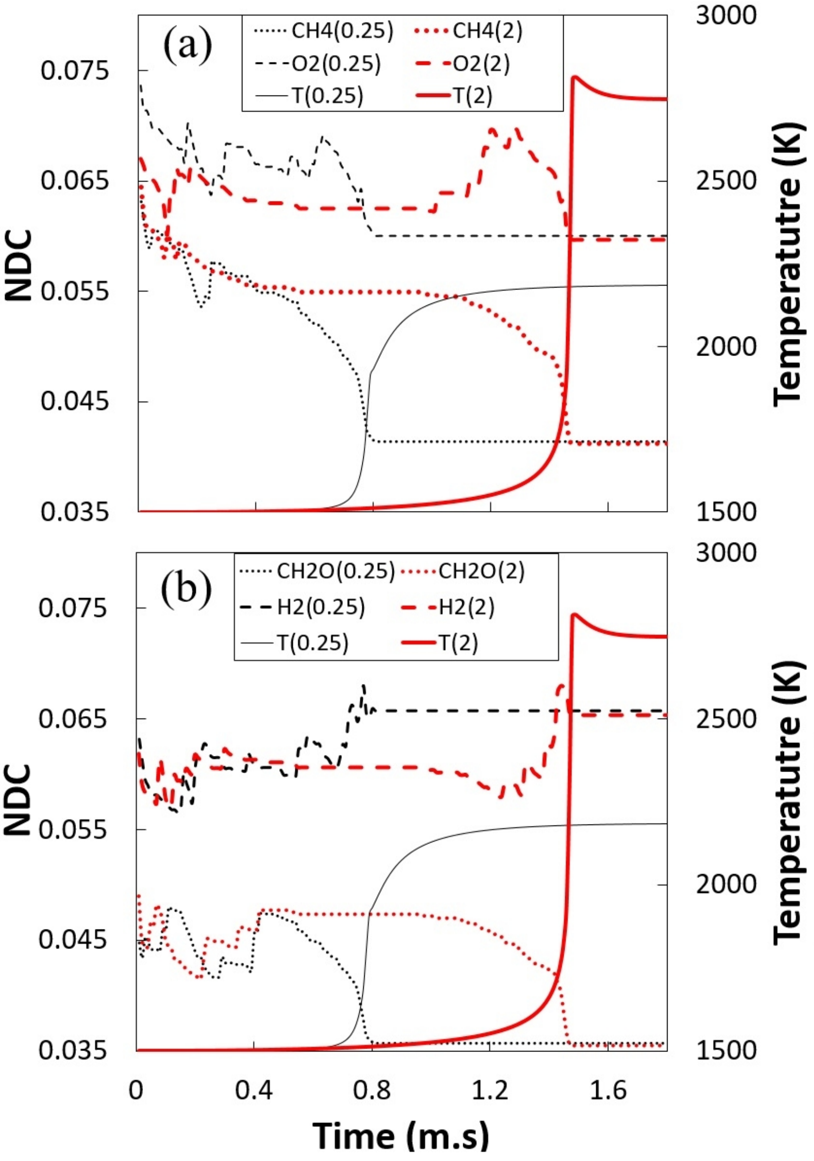
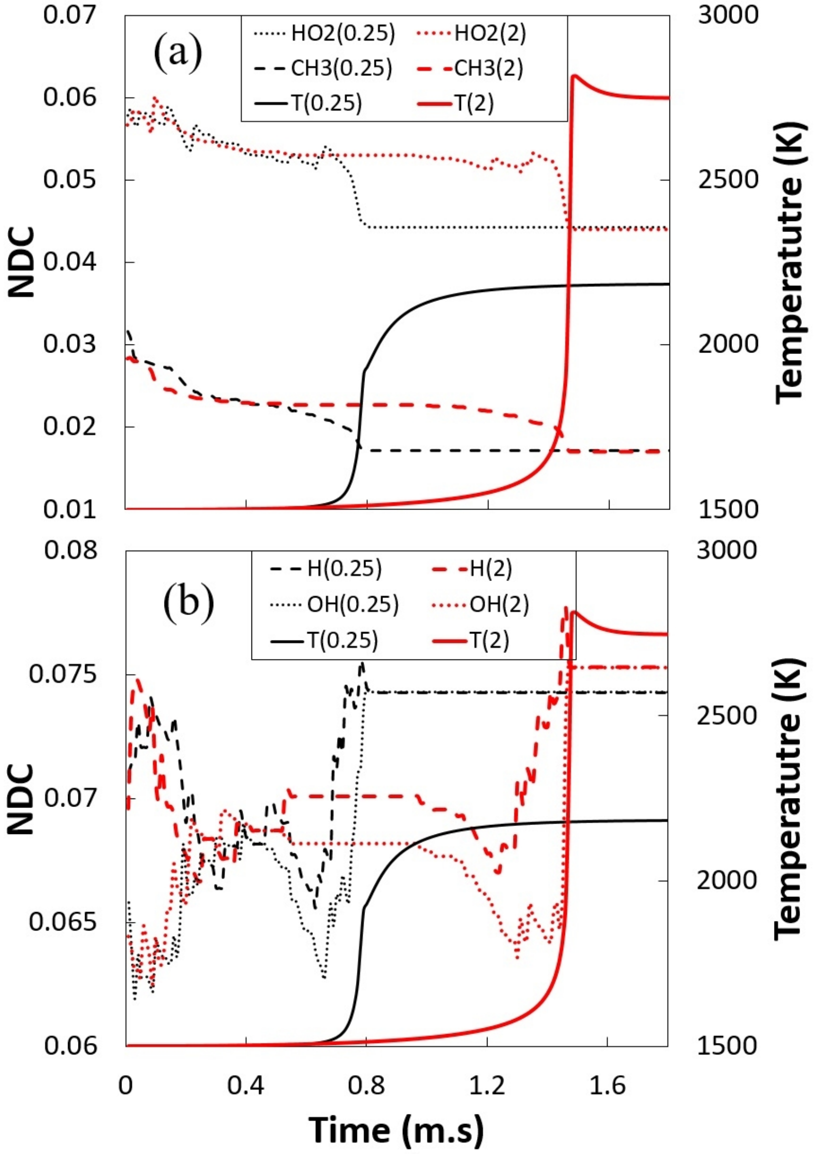


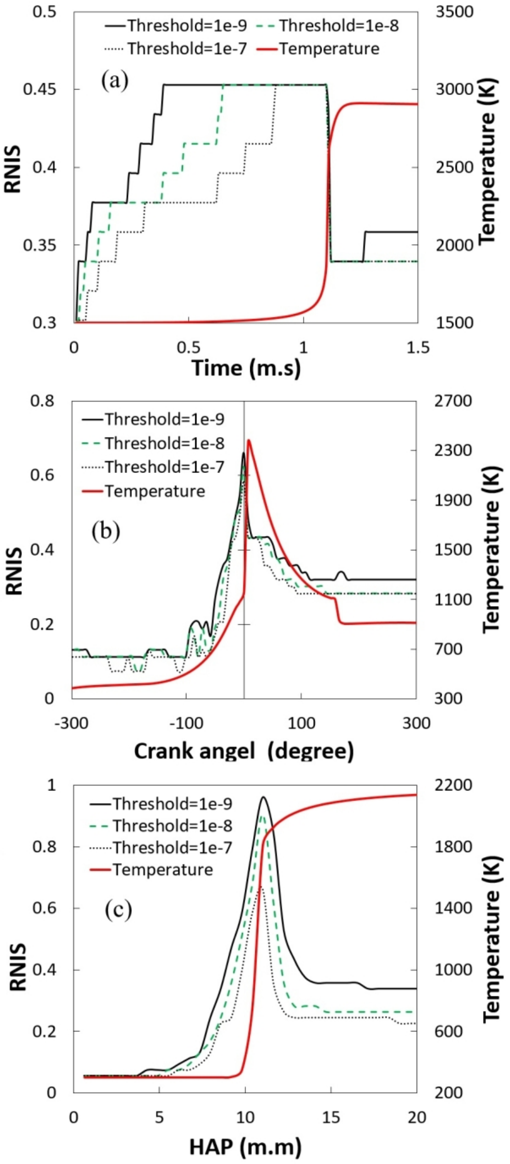
A part of CRN graph generated automatically at *t*= 1 ms for methane/air ignition process under the RCM combustion conditions of *T*= 1500 K, *p*= 1 bar and Φ= 1.



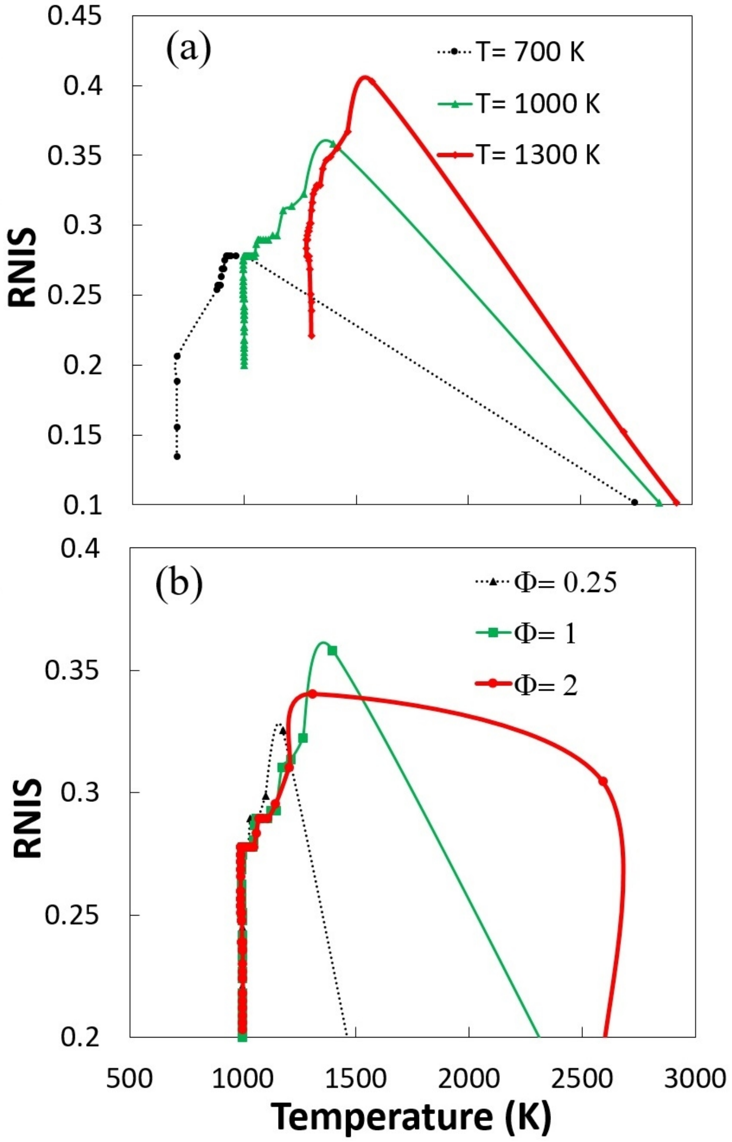
Timing history of temperature and NDC for some stable species of methane/air fueled RCM at combustion conditions of *T*= 1500 K, *p*= 1 bar and Φ= 0.25 and 2.



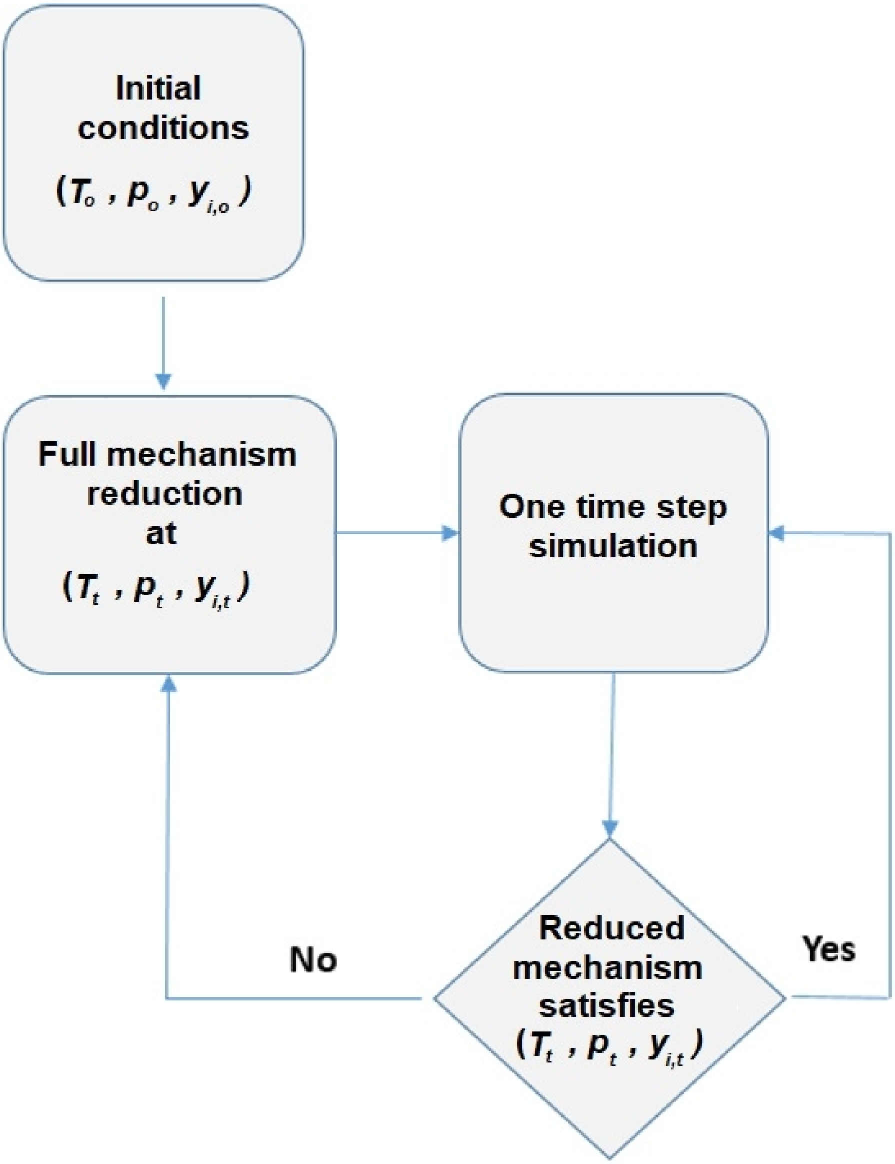
Timing history of temperature and NDC for representative radicals of low-intermediate and high temperature chemistries of methane/air fueled RCM at combustion conditions of *T*= 1500 K, *p*= 1 bar and Φ= 0.25 and 2.



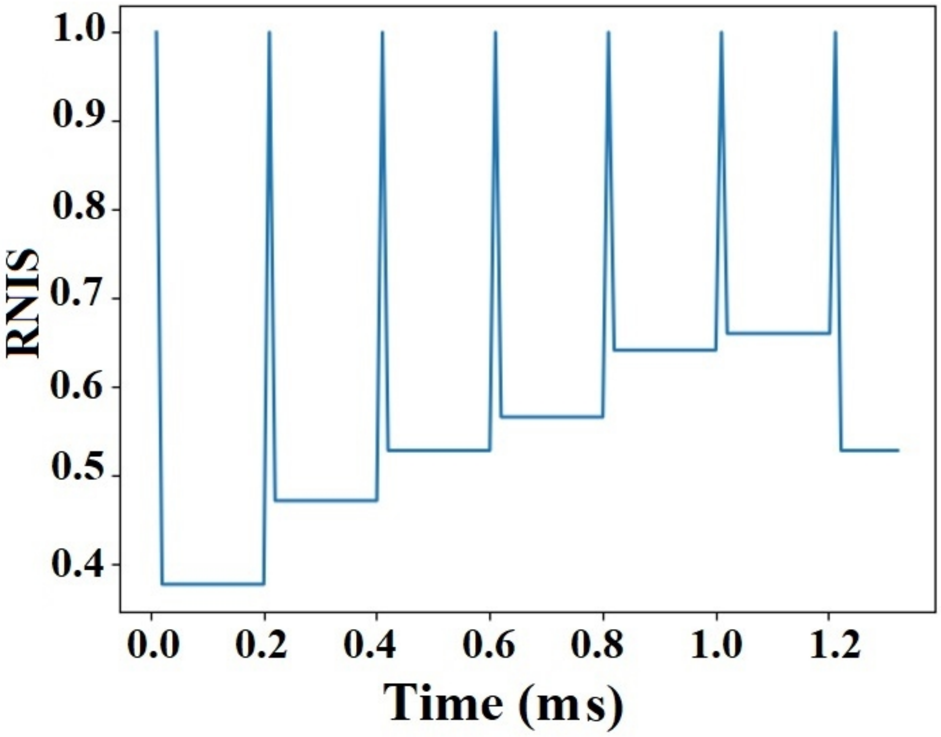
RNIS in function of time, crank angle and HAB for methane/air fueled RCM (a): *T*= 1500 K, *p*= 1 bar and Φ= 1, HCCI engine (b): *T*= 1500 K, *p*= 1 bar, engine speed= 600 rpm, compression ratio= 17 and Φ= 1 and laminar premixed flame (c): *T*= 300 K, *p*= 1 bar and Φ= 1, respectively.



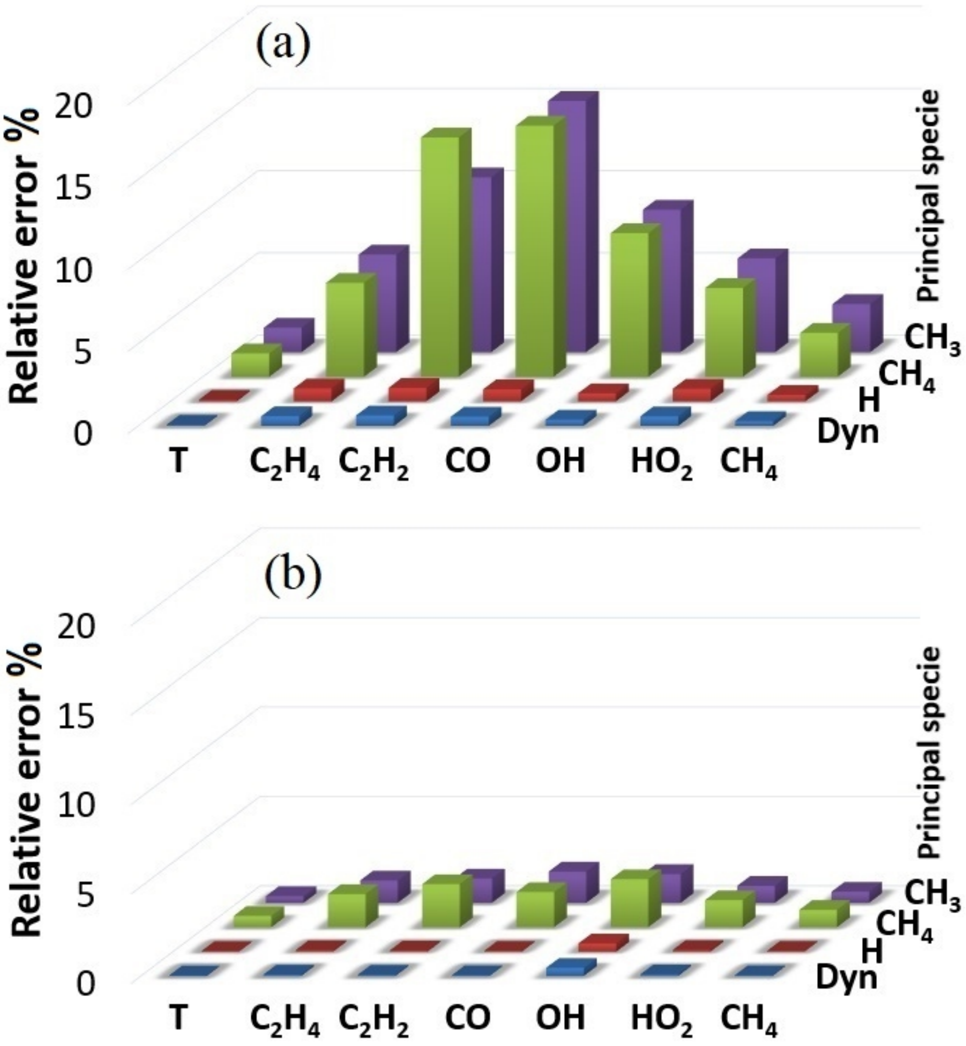
RNIS in function of temperature history of *n*-heptane/air fueled RCM oxidation conditions for different initial mixture temperatures (a): *T*= 700, 1000 and 1300 K, *p*= 1 bar and Φ= 1, and different equivalence ratios (b): Φ= 0.25, 1 and 2, *T*= 1000 K and *p*= 1 bar.



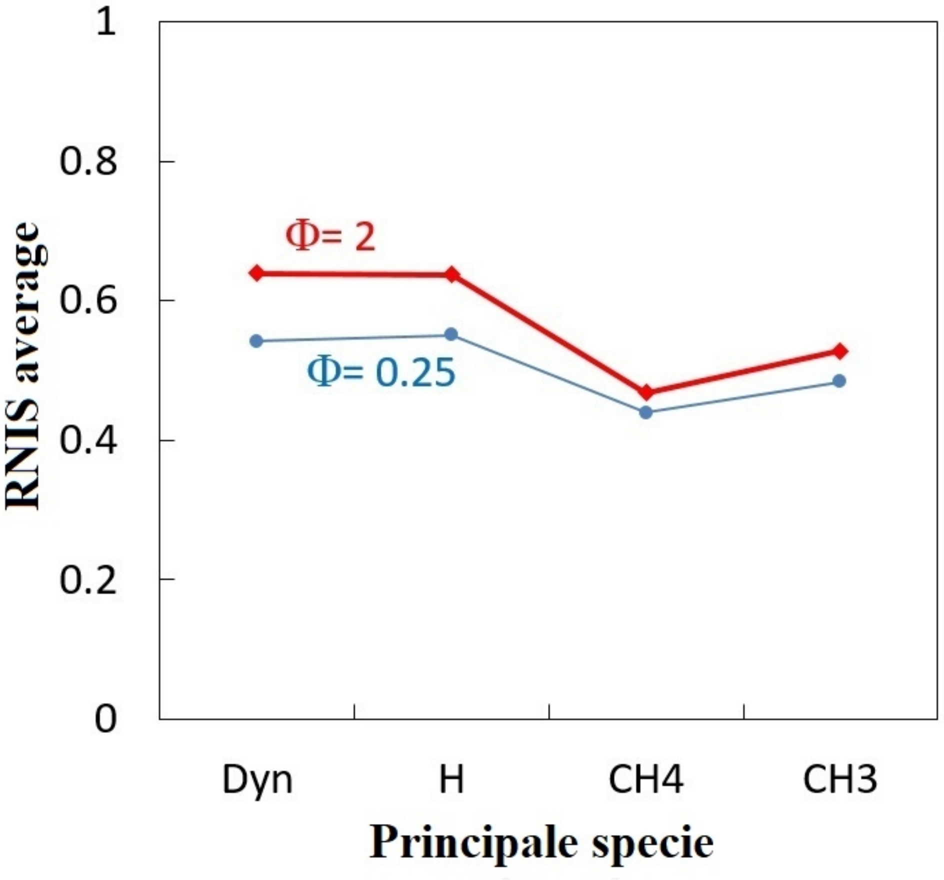
DAC implementing approach diagram.



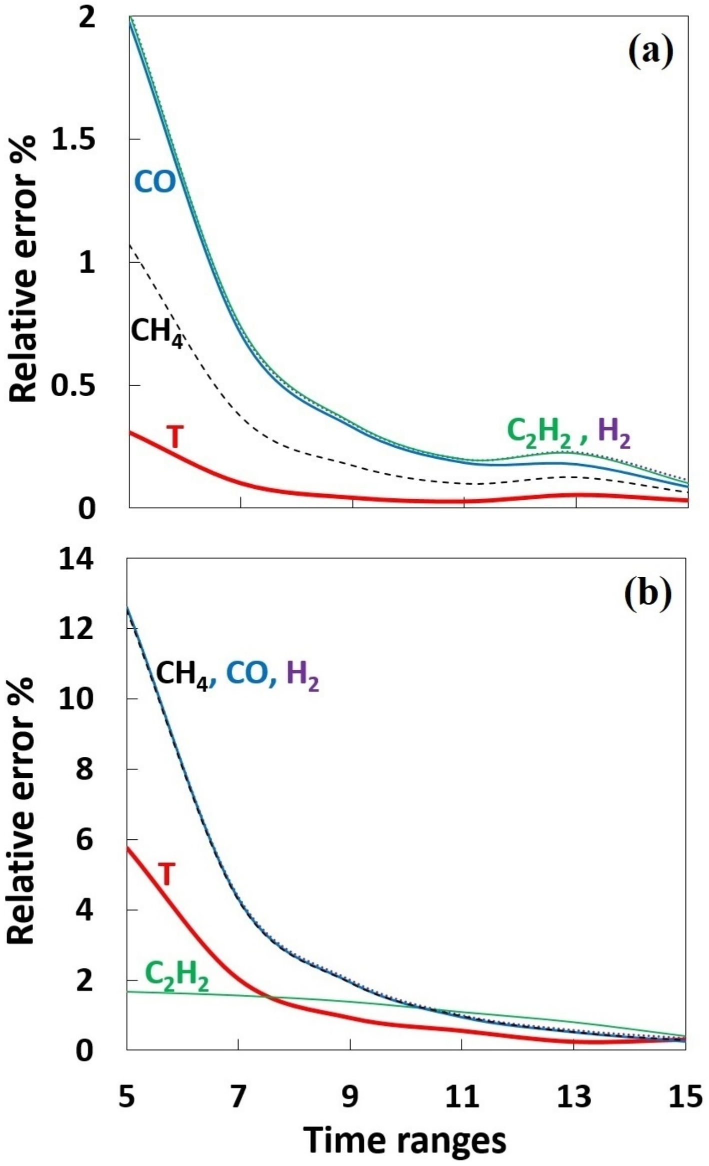
Timing history of the reduced mechanisms RNIS implemented by the DAC approach, ε= 1.10$^{-7}$ and $N_t$= 7, for methane/air fueled RCM at combustion conditions of *T*= 1500 K, *p*= 1 bar and Φ= 1.



Relative error % in function of dynamic (Dyn) and predetermined principal species selection, $CH_4$, $CH_3$ or H, of DAC application conditions of $\varepsilon = 1.10^{-7}$ and $N_t = 11$, of the predicted time history values of temperature and species concentration for methane/air fueled RCM at combustion conditions of $T = 1500$ K, $p = 1$ bar and $\Phi = 0.25$ (a) and 2 (b).



RNIS average in function of dynamic (Dyn) and predetermined principal species selection, $CH_4$, $CH_3$ or H, of DAC application conditions of $\varepsilon = 1.10^{-7}$ and $N_t = 11$, for the simulations of methane/air fueled RCM at combustion conditions of $T = 1500$ K, $p = 1$ bar and $\Phi = 0.25$ and 2.



Relative error % in function of time ranges number used by DAC application, ε= 1.10$^{-7}$ and dynamic principal species selection, of the predicted time history values of temperature and species concentration for methane/air fueled RCM at combustion conditions of $T$= 1500 K, $p$= 1 bar and Φ= 0.25 (a) and 2 (b).