Preliminary Study on Reduced Chemical Mechanisms for Hydrogen–Air Combustion

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Abstract — The combustion of hydrogen with air as a promising method for converting energy into zero-carbon power production and propulsion systems is gaining worldwide appreciation. The complex chemical kinetics involved in the high reactivity and radical-driven nature of hydrogen flames, however, are usually described by detailed mechanisms that include 20–21 elementary reactions and 8–10 species. Such methodologies are also computationally very expensive, and often uneconomical on complex simulations such as computational fluid dynamics (CFD), flames analysis or ignition modelling. Accurate modeling is made possible by reduction chemistry, which is the methodical simplification of chemical reaction pathways with less computational overhead. In this article, a very simple review of the reduction chemistry directed to hydrogen-air ignition systems, the need of reduction chemistry, classification, and step-by-step explanation of the key reduction approaches mentioned in literature, such as skeletal, quasi-steady-state (QSSA), intrinsic low-dimensional manifold (ILDM) based methods, and directed relation graph (DRG) based approaches have been discussed.

Keywords: Reduced Mechanism, Reduction Chemistry, Hydrogen Combustion, Green Energy

I. INTRODUCTION

The possibility of air hydrogen combustion as clean renewable energy is turning it important especially with regard to decarbonizing gas turbine systems and propulsion technologies [1, 2]. Complex chemical dynamics involving many elementary processes and reactive intermediates must be represented in order to accurately characterize hydrogen–air combustion [3]. However, even though they are extremely precise, complex reaction mechanisms are frequently computationally costly and unfeasible for use in large-scale simulations like computational fluid dynamics (CFD) of combustors [4]. This calls for the creation of simplified chemical processes, which seek to drastically reduce computational requirements while maintaining crucial chemical integrity [5].

A number of basic elementary steps and reactive species, including H, O, OH, HO_2, H_2O_2, and others, are involved in the hydrogen-air combustion reaction [6]. To fully capture the dynamics of combustion with all possible chemical routes, a thorough mechanism, is developed by Li et al. (2004), may have dozens of reactions and species [7]. It might be computationally very expensive and even impossible, however, to resolve such complex mechanisms in simulation, especially at CFD level. In this sense, reduction chemistry is the process of determining and removing less important species and reactions, building a more compact, computationally effective model, while preserving enough precision for the intended use (e.g., pollutant production, flame propagation, ignition delay prediction) [5].

Because detailed mechanisms frequently require solving stiff ordinary differential equations (ODEs) with dozens of species and reactions, which greatly raises the computational cost, one of the main reasons for reducing detailed chemical kinetic mechanisms is computational efficiency [4, 8]. Large kinetic models also present numerical stability challenges since they frequently show stiffness and convergence problems in simulations [9]. From a view of practical engineering, capturing particular macroscopic properties like flame speed or ignition delay is the main goal of many combustion applications, including gas turbines and internal combustion engines [8]. Therefore, reduction solutions that are application-focused are adequate and frequently favored. Additionally, less mechanisms allow for quicker design iterations, which speed up the development cycle of combustion systems by facilitating the execution of parametric studies and optimization loops.

II. LITERATURE REVIEW

Fig. 1 shows the gradual development of study methods related to combustion chemistry in last century [10]. Various reduction mechanisms have been studied to enable effective simulation of hydrogen–air combustion. In order to achieve the reduction of complex chemical pathways in preserving important combustion properties, Huang et al. (2005) [5] have suggested a systematic method to lump that involves sensitivity analysis, skeletal reduction and principal component analysis. Their approach demonstrated the ability to preserve valid predictions of ignition delay and the flame-speed, thus they were appropriate to apply to the computational models of combustion. In order to facilitate the appropriate modeling of reduction, as well as pressure-independent reaction kinetics of recombination reaction $H + O_2 + M \rightarrow HO_2 + M$ were experimentally investigated by Bates et al. (2001) [11]. Fall-off characteristics at high temperatures and at high pressures were determined by means of shock tube diagnostics. The effects of third-body interactions were illuminated by the rate constant calculated with RRKM (Rice Ramsperger Kassel Marcus) and Troe approximations and especially when under high pressure environment as in the case of gas turbine operating conditions. Hessler (1998) [12], developed a way to calculate microcanonical rate constants by means of inverse Laplace transformation from macroscopic Arrhenius relations. Another optimization of reduction chemistry was made possible due to his theoretical work. This has contributed in bridging the accuracy of detailed models in kinetics with the problems of reduced models by allowing the calculation of energy-resolved cross sections and errors.

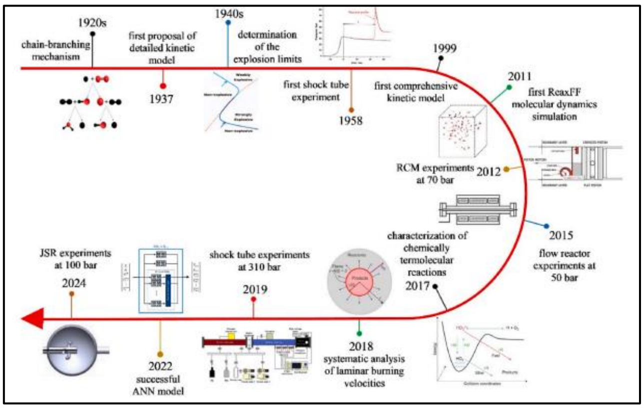

Fig. 1: The gradual development of study methods related to combustion chemistry [10].

Strohle and Myhrvold (2006) [13] also attempted reduction mechanisms in combustion of lean hydrogen on high pressure. This made it easier to simplify the hydrogen kinetics through straight forward computer framework still preserving important flame structure and as a result computational efficiency was increased in the extreme high-pressure conditions. Davis et. al. (2005) [14] have recently formulated an optimized skeletal mechanism of H_2-CO combustion including a re-evaluated set of reaction paths and mass updated rate coefficients. The model has shown better predictive skills of ignition delay and flame speed under a variety of thermodynamic states. The important considerations regarding the CO reaction paths in the scenario of hydrogen-rich combustion was considerably justified by the outcome of their validation process. Through CFD simulation in ANSYS CFX, Zhukov (2012) [15] carried out a detailed verification and validation of different hydrogen oxidation kinetic schemes as well as a testing of its various schemes. Comprehensive and simplified models were compared using their forecasts of flame velocity and ignition delay. Special consideration was given to the mechanisms that provide a high degree of accuracy and minimal computational expenses. The conclusion was that one would be able to substantially shorten the simulation time using good calibrated skeletal models without reducing the reliability of the predictions.

	Reactions	A	n	E
	Chain Reactions H_2/O_2			
1	$H + O_2 \rightarrow O + OH$	3.55×10^{15}	-0.41	16.6
2	$O + H_2 \rightarrow H + OH$	5.08×10^{4}	2.67	6.29
3	$H_2 + OH \rightarrow H_2O + H$	2.16×10^{8}	1.51	3.43
4	$O + H_2O \rightarrow OH + OH$	2.97×10^{6}	2.02	13.40
	Dissociation/Recombination Reactions H_2/O_2			
5	$H_2 + M \rightarrow H + H + M^a$	4.58×10^{19}	-1.40	104.38
	$H_2 + He \rightarrow H + H + He$	5.84×10^{17}	-1.10	104.38
	$H_2 + Ar \rightarrow H + H + Ar$	5.84×10^{17}	-1.10	104.38
6	$O + O + M \rightarrow O_2 + M^a$	6.16×10^{15}	-0.50	0.0
	$O + O + Ar \rightarrow O_2 + Ar$	1.89×10^{13}	0.00	-1.79
	$O + O + He \rightarrow O_2 + He$	1.89×10^{13}	0.00	-1.79
7	$H + O + M \rightarrow OH + M^a$	4.71×10^{18}	-1.00	0.0
8	$H + OH + M \rightarrow H_2O + M^b$	3.80×10^{22}	-2.00	0.0
	HO_2 Formation and Consumption			
9	$H + O_2 + M \rightarrow HO_2 + M^c$	6.37×10^{20}	-1.72	0.52
	$H + O_2 + M \rightarrow HO_2 + M^d$	$9.04 x 10^{19}$	-1.50	0.49
10	$HO_2 + H \rightarrow H_2 + O_2$	1.66×10^{13}	0.00	0.82
11	$HO_2 + H \rightarrow OH + OH$	7.08×10^{13}	0.00	0.30
12	$HO_2 + O \rightarrow OH + O_2$	3.25×10^{13}	0.00	0.00
13	$HO_2 + OH \rightarrow H_2O + O_2$	2.89×10^{13}	0.00	-0.50
	H_2O_2 Formation and Consumption			
14	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2^e$	4.20×10^{14}	0.00	11.98
	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	1.30×10^{11}	0.00	-1.63
15	$H_2O_2 + M \rightarrow OH + OH + M^f$	1.20×10^{17}	0.00	45.50
16	$H_2O_2 + H \rightarrow H_2O + OH$	2.41×10^{13}	0.00	3.97
17	$H_2O_2 + H \rightarrow H_2 + HO_2$	4.82×10^{13}	0.00	7.95
18	$H_2O_2 + O \rightarrow OH + HO_2$	9.55×10^{6}	2.00	3.97
19	$H_2O_2 + OH \rightarrow H_2O + HO_2^e$	1×10^{12}	0.00	0.00
	$H_2O_2 + OH \rightarrow H_2O + HO_2$	5.8×10^{14}	0.00	9.56

Table 1: Full Reaction Mechanism (H_2/O_2). Units: cm^3 mol sec kcal K [7]

Abundant study has been done on the Chain-branching processes which dominate when temperature is high and pressure is low in the H_2/O_2 system. There are still reaction involving the intermediate species such as the hydrogen peroxide (H_2O_2) and the hydroperoxyl (HO_2) reactions which are considered to be relatively not well understood.

Kinetic investigation of hydrogen combustion was significantly enhanced by the one of the first works of Mueller et al. [16], who confirmed a complete 19-reaction mechanism and revised the rate constants with consideration of new thermochemical data using a Variable Pressure Flow Reactor (VPFR). It was discovered to be inadequate in predicting flame speeds in $H_2/O_2/He$ blends at pressures of up to 20 atm [7] even though it encompassed key features of radical forming, that is, the presence of predominant radical formation in the form of atomic hydrogen.

A revised hydrogen combustion mechanism was developed by Li et al. [7] in order to overcome these constraints. It kept the 19 reversible reactions listed in Table 1 but included new thermodynamic information and more experimental confirmations. Their research expanded the use of reduced mechanisms in a variety of experimental setups, such as laminar premixed flames and shock tubes. This wholesome revision also incorporated the differences in the enthalpy of formation of the hydroxyl (OH) radical supported by the calorimetric experiments [12], and more productive factors of the third-body species including He, Ar, and H2, H2O. These advancements have underlined the fact that care should be taken to ensure that the mechanisms of reduction are kept current as a mechanism of enhancing their predictive capacity within the varied combustion regimes [17]. In total the development of hydrogen-air combustion reduction mechanisms has not yet struck a proper equilibrium between computational cost-effectiveness and chemical precision.

This search is a conceptual overview of reduction chemistry of the hydrogen combustion systems, explaining the motivation and techniques associated with the system and outlining the primary progresses made in the study with reference to the experimentally proven mechanisms.

III. Methodologies for Hydrogen-Air Mechanism Reduction

There have been found four types (Table 2) of parametric reductions of the hydrogen-air mechanism in the literature. Each method provides a different trade-off between accuracy, automation, and range of applicability, as described in following.

A. *Skeletal Reduction*

Mostly for computational fluid dynamics (CFD) applications and for simplifying hydrogen combustion mechanisms, it is one of the widely implemented methods. The first step of the procedure is to define all the relevant operating condition of the process like pressure, temperature, equivalence ratio etc. Under specified operating condition, simulations with complete chemical mechanisms—like that given by Li et al. [7] and widely accepted by chemical community are carried out to study important combustion parameters such as laminar flame speed, and ignition delay time etc. Then by applying species importance criteria chemically unimportant species are determined usually with constraints like mole fractions less than 10^{-6} [18]. By removing such species, with their accompanying reactions systematically a reduced but representative skeletal mechanism can be obtained. The last step involves validation of result obtained through reduced mechanism pertaining to key combustion parameters with the results from the original detailed mechanism. In case of elevated temperatures, species such as HO_2 and H_2O_2 can often be neglected without conceding the accuracy of ignition delay predictions by more than 5% [19]. In this way a balance between computational efficiency and chemical reliability can be obtained making it especially attractive for high-fidelity engineering simulations.

Method	Foundation	Common Tools
Skeletal Reduction	Threshold-based species pruning	CHEMKIN, Cantera
QSSA	Time-scale based species elimination	Analytical, COPASI
ILDM / CSP	Timescale separation via Jacobian eigen analysis	CSP Toolbox
DRG-based (DRG, DRGEP, DRGASA)	Graph theory with sensitivity metrics	DRGEP, YARC

Table 2: Parametric reductions Method as per Literature

B. *Quasi-Steady State Approximation (QSSA)*

The QSSA is more effective when certain radical intermediates react faster than those of the major stable species involved in reaction on timescales [20]. In case of hydrogen air combustion, the highly reactive intermediates like OH, O, Ho etc. are present in typical quasi steady state species [6]. Here also the first step starts with identifying the fast-reacting intermediates, where it is assumed that it is maintaining a dynamic equilibrium during the chemical reaction. By setting the time derivative of their concentration dC/dt to zero and imposing a steady state condition on these species, it can be presented mathematically and the resulting numerical equations can be solved to express the concentration of quasi-steady-state species in terms of non-quasi-steady-state species. Then it is substituted in to remaining set of ordinary differential equations. In this way the dimensionality of the kinetic system is reduced resulting in improved computational efficiency [21]. But the validity of QSSA is highly dependent on the condition of specific reaction. In case QSS species play an important role in determining important combustion properties, e.g. ignition delay or extinction limits [19], this can cause poor predictions. Therefore, requirement of accurate validation by comparing it with the detailed combustion reaction arise for reliability and accurateness of the result.

C. *Intrinsic Low-Dimensional Manifold (ILDM) and Computational Singular Perturbation (CSP)*

The Intrinsic Low-Dimensional Manifold (ILDM) and Computational Singular Perturbation (CSP) methods are technics for advanced reduction mechanism. It is based on the separation of chemical timescales, for simplifying complex chemical kinetic systems which is done by offering a mathematically rigorous framework. By constructing the Jacobian matrix of the governing species equations, it captures the local linearized behavior of the reaction system. By eigenvalue decomposition, the dynamics are decomposed into the fast and slow modes; the fast modes, with fast decaying transient are discarded, and the slow modes establish the manifold on which the system is projected [23]. The ILDM approach, introduced by Maas and Pope [24], identifies a low-dimensional surface in composition space that will encompass the essential chemical evolution. In the same way, the CSP method, developed by Lam and Goussis [25], allows the system to be projected onto a reduced set of equations maintaining the dominant chemical behavior by decomposing the system with time scale base transformation. This simplified form is subsequently incorporated in CFD or reactor models, at much reduced computational cost at run time. However, both ILDM and CSP require large amount of pre-processing, since they involve iterative calculation of Jacobians and eigenvalue analysis of a wide range of thermochemical states and therefore, it is computationally intensive before deploying [20]. Nevertheless, they have such properties as accurate results and the closeness of the burn model to reality, which makes their use for high-fidelity combustion simulations interesting.

D. Directed Relation Graph (DRG)

The Directed Relation Graph (DRG) family of methods—including its extensions DRG with Error Propagation (DRGEP) and DRG with Sensitivity Analysis (DRGASA)—are graph-theoretic approaches widely employed for the reduction of detailed chemical kinetic mechanisms. These methods model species as nodes in a directed graph, where the edges are weighted based on normalized reaction rate dependencies that quantify the coupling strength between species [3]. Figure 1 shows the typical relations between the species in a DRG. The arrow indicates the direction of dependence of one species on another. The width of arrow indicates the strength of the dependence [22].

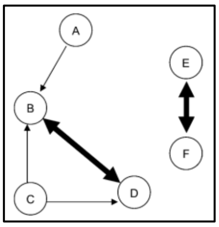

Fig. 2: A characteristic relation of the species indication using directed relation graph [22].

The reduction procedure begins by selecting a set of target species, typically major species such as H_2, O_2, and H_2O, whose accurate prediction is essential. An interaction graph is then constructed by computing coupling coefficients from the reaction fluxes, and a threshold parameter (ε) is applied to eliminate species deemed unimportant based on their weak interactions with the target species. The DRGEP method improves upon DRG by accounting for error propagation along indirect paths, thereby enhancing the robustness of species selection [22]. Further refinement is achieved in DRGASA, which incorporates sensitivity analysis to retain species and reactions that significantly affect target quantities, even if they exhibit weak direct couplings [18]. These techniques have been particularly effective in hydrogen–air combustion, where reduced mechanisms with as few as 7 - 9 species and approximately 10 reactions can accurately reproduce ignition delays and flame speeds. For example, Lu and Law [18, 22] successfully applied DRGEP to reduce the detailed Li et al. mechanism to a 7-species skeletal model with negligible loss in accuracy for ignition delay predictions. The DRG-based methods strike an excellent balance between computational efficiency and fidelity, making them well-suited for large-scale CFD simulations and combustion system optimization. Table 3 shows the Comparative Evaluation of these four methods.

Feature	Skeletal	QSSA	ILDM/CSP	DRG-based
Automation	Low	Medium	Medium	High
Physical Rigor	Low	Medium	High	High
CFD Readiness	High	Medium	Medium	High
Best applied for	Lean flames	Post-flame zones	Autoignition	General hydrogen combustion

Table 3: Comparative Evaluation

IV. GLOBAL TO SKELETAL MECHANISMS

A. Base Mechanism

The full mechanism by Li et al. [7] showing 9 species and 19 elementary reactions as per Table 1 is generally considered for reduction purpose. The reduction is performed using appropriate method described in Table 2, followed by sensitivity analysis to retain key reactions affecting ignition delay and laminar flame speed.

B. One-Step Global Mechanism

The one-step global mechanism represents the overall combustion reaction of hydrogen as a single irreversible step, typically written as:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad (1)$$

This process fails to solve intermediate species and elementary reactions. It is mostly applied in engineering practice where simple flame propagation or rate of heat released is called upon like when modeling a flamelet or a simple burner [8]. It does not however, capture ignition delay, formation of NO_x or radical chemistry [26]. Using an Arrhenius-type rate expression fitted to empirical data [27] the reaction rate is modeled. It is used for fast estimation of combustion performance in systems where chemical kinetics are not dominant.

C. Two-Step Global Mechanism

The two-step mechanism introduces a fuel oxidation stage followed by a heat release or recombination step. An example is [28]:

$$H_2 + O_2 \rightarrow 2OH \quad (2)$$

$$2OH + H_2 \rightarrow 2H_2O \quad (3)$$

The level is global in nature but starts considering radical pool formation, the result of which, in the reasonable state, made the ignition delay time prediction better than the one-step model by a little bit. This makes better prediction of reactions rate, sensitive to the temperature, but not reliable to different pressure conditions [28]. It is however still inadequate to transient and turbulent flows involving reactive flow computations in which intermediate species (HO_2, H_2O_2, etc.) are important. It is used in simulation of easy-to-understand models of ignition and teaching demonstrations.

D. Three-Step Mechanism

A three-step mechanism further introduces radical propagation and chain branching, such as [29, 30]:

$$H_2 + O_2 \rightarrow OH + OH \quad (4)$$
$$OH + H_2 \rightarrow H_2O + H \quad (5)$$
$$H + O_2 \rightarrow OH + O \quad (6)$$

The formulation represents key chain-branching and propagation phenomena in hydrogen oxidation and may be used to reasonably estimate flame velocities and ignition delays in limited conditions. It also introduces significant species such as H, OH, and O which control flame propagation. However, low-temperature oxidation and pressure effects are still not resolved[29, 30]. It is moderate-accuracy modeling for validation of reduced flame behavior or control strategies.

E. Four-Step Mechanism

A four-step mechanism encompasses a chain termination or quenching step, allowing limited modeling of reaction completeness and flame extinction. An example is [29]:

$$H_2 + O_2 \rightarrow OH + OH \quad (7)$$
$$OH + H_2 \rightarrow H_2O + H \quad (8)$$
$$H + O_2 \rightarrow OH + O \quad (9)$$
$$H + OH + M \rightarrow H_2O + M \quad (10)$$

The third-body recombination is introduced in the fourth step, which improves predictions in gas turbine like high-pressure environments. But especially in case of low temperatures and high pressures scenarios there is a lack of representation of peroxy radicals (HO_2, H_2O_2) critical in ignition and extinction phenomena, [26]. For combustion systems operating near atmospheric to moderate pressures, it can be used.

F. Five-Step Mechanism

The five-step mechanism adds peroxide chemistry, improving accuracy in ignition delay predictions. An example is:

$$H + O_2 \rightarrow HO_2 \quad (11)$$
$$HO_2 + H \rightarrow 2OH \quad (12)$$
$$OH + H_2 \rightarrow H_2O + H \quad (13)$$
$$H + OH + M \rightarrow H_2O + M \quad (14)$$
$$H_2 + O_2 \rightarrow H + HO_2 \quad (15)$$

These are low temperature branching and quenching steps and these can be used to model auto ignition and flame extinction at higher combustion pressures in hydrogen, in particular engines and reheat combustors. In some model NOx can be predicted using tracking of HO_2 like radicals. It appears in autoignition research, and in medium-fidelity [31] CFD modeling of hydrogen air CFD simulation.

G. Six-Step Mechanism

The six-step mechanism includes additional species like H2O2 to improve accuracy for low temperature or high-pressure conditions. An example is:

$$H_2 + O_2 \rightarrow 2OH \quad (16)$$
$$OH + H_2 \rightarrow H_2O + H \quad (17)$$
$$H + O_2 + M \rightarrow HO_2 + M \quad (18)$$
$$HO_2 + H \rightarrow 2OH \quad (19)$$
$$H + H + M \rightarrow H_2 + M \quad (20)$$
$$HO_2 + HO_2 \rightarrow H_2O_2 + O_2 \quad (21)$$

These are pressure- and temperature- sensitive, which enhances the reliability of models in advanced combustors. Just like in the four-step reduced reaction mechanism, but keep H2O2 reactions so as to capture peroxide reaction chemistry at low temperatures [31]. Rates need to be calibrated to the inert conditions of ignition delay and flame speed.

H. Eight-Step Skeletal Mechanism

By retaining 8-12 critical reactions without extensive lumping it is a simplified version of detailed mechanism. They are not as reduced as the mechanisms above but are simpler than full mechanisms. It includes key branching, propagation, termination and peroxide reactions without QSSA reductions [4]. An example is:

$$H + O_2 \rightarrow OH + O \quad (22)$$
$$OH + H_2 \rightarrow H_2O + H \quad (23)$$
$$H + O_2 + M \rightarrow HO_2 + M \quad (24)$$
$$HO_2 + H \rightarrow 2OH \quad (25)$$
$$H + H + M \rightarrow H_2 + M \quad (26)$$
$$HO_2 + HO_2 \rightarrow H_2O_2 + O_2 \quad (27)$$
$$H_2 + O \rightarrow OH + H \quad (28)$$
$$OH + OH \rightarrow H_2O + O \quad (29)$$

V. Results and Discussion

In order to accurately and efficiently predict hydrogen air combustion, reduction chemistry is essential. In this study various reduction mechanisms, from simple global one-step models to advanced skeletal mechanisms were reviewed, highlighting their applicability and limitations. Although global and few step mechanisms have computational advantages, they lack the accuracy required to represent fine scale combustion phenomena. On the contrary, reduced-order models of skeletal mechanisms, which are obtained using models such as QSSA, DRGEP, ILDM, preserve important chemical dynamics but with much simpler complexity and lend themselves to CFD and high-fidelity use.

VI. Conclusions

Mechanism	Steps	Species	Accuracy	Applications
One-Step	1	H_2, O_2, H_2O, N_2	Low	Simple engineering models
Two-Step	2	H_2, O_2, H_2O, H, M	Moderate	Basic CFD with radical formation
Three-Step	3	H_2, O_2, H_2O, H, OH, M	Moderate	Flame speed, ignition delay
Four-Step	4	H_2, O_2, H_2O, H, OH, HO_2, O, M	Moderate–High	Flame structure, extinction limits
Five-Step	5	H_2, O_2, H_2O, H, OH, HO_2, M	High	Low-temp chemistry, detailed kinetics
Six-Step	6	H_2, O_2, H_2O, H, OH, HO_2, H_2O_2, M	High	High-pressure, low-temp ignition

Skeletal	8 - 12	H_2, O_2, H_2O, H, O, OH, HO_2, H_2O_2, M	Very High	Detailed simulations, advanced CFD modelling

Table 4: Comparison of Various Mechanism

The mechanism (Table 4) to be applied will be determined by the necessary tradeoff between the computational cost and physical accuracy. As hydrogen advances to become the leading clean energy carrier; for advancing reliable and scalable combustion technologies, robust reduced mechanisms will be essential.

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