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Macrokinetic Behavior of Hydrogen Combustion under High Pressure with Turbulence and Thermal Inhomogeneity

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Keywords:

Hydrogen combustion; Microkinetic; Ignition delay; Turbulence; Temperature gradient; High pressure; Radical concentration; Numerical modelling.

Highlights:

- A temperature gradient of 300 K reduced the ignition delay to 0.26 seconds at 10 MPa.
- Radical OH concentrations increased to 3.9×10^{-4} mol/mol in locally overheated turbulent zones.
- The adapted global kinetic model achieved an error of less than 8% across various combustion regimes.

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Abstract: This study investigates how turbulence intensity and temperature gradients affect the macroscopic kinetics of hydrogen-air combustion at supercritical pressures from 10 to 20 MPa. A series of high-precision experiments was conducted in a custom-designed high-pressure combustion reactor with a controllable thermal field and adjustable turbulent-flow generation. The induction period for spontaneous ignition was measured under various turbulence regimes and temperature distributions. Increasing turbulence intensity from 0% to 20% reduced the induction period from 0.71 s to 0.39 s, and imposing a linear temperature gradient of 300 K over 15 cm further decreased it to 0.26 s. The maximum radical concentrations of H and OH were 3.5×10^{-4} and 3.9×10^{-4} mol/mol at 20 MPa and 1000 K, indicating enhanced chain-reaction activity in locally overheated regions. Numerical simulations using a modified global kinetic model deviated by less than 8% from the experimental data. The findings support the development of improved macrokinetic models suitable for engineering applications involving hydrogen combustion at high pressures with complex thermal and flow fields.

1. INTRODUCTION

In recent decades, sustainable energy development has been central to global efforts to ensure environmental and technological security. A critical aspect of this process has been the transition from traditional hydrocarbon fuels to alternative energy sources with low carbon footprints and high specific energy efficiency. In this context, hydrogen has attracted particular attention as the most promising future energy carrier. Its combustion produces no carbon dioxide, and its calorific value is 120 MJ/kg, approximately three times that of typical hydrocarbons such as methane or gasoline [1-3]. Hydrogen energy is actively considered in the development roadmaps of the EU, the USA, Japan, South Korea and China. By 2023, global investment in hydrogen technologies had exceeded 20 billion US dollars, and, according to IEA forecasts, global hydrogen consumption could reach 200 million tons per year by 2030 [4,5]. However, despite the potential benefits, the large-scale introduction of hydrogen faces numerous daunting scientific and technical challenges. One of these challenges is to ensure stable and predictable hydrogen combustion in the conditions typical of modern power plants, for example, in the combustion chambers of gas turbine engines, direct combustion plants, detonation engines, as well as high-load energy systems with forced pressure [6-8]. A characteristic feature of these systems is to operate at pressures exceeding 10 MPa, in the presence of strong temperature gradients and developed turbulence. Such conditions have a critical impact on the ignition process and combustion stability, which, in turn, determine the safety and efficiency of the entire plant [9-11]. To date, two main approaches are used to model hydrogen combustion processes: detailed kinetic mechanisms (DCM), which include dozens of elementary reactions involving active radicals, and simplified global kinetic models (macrokinetics) designed for engineering calculations. The first approach achieves high modelling accuracy, particularly for describing the initial stages of oxidation, induction periods, and radical distributions, but its computational complexity is exceptionally high [12-14]. For example, in a hydrogen-oxygen mixture, modern DCM can contain 30 to 60 elementary reactions involving more than 10 components, including H, OH, O, HO₂, H₂O₂, and others. Solving a system of 60 stiff differential equations at high pressures and variable thermodynamic parameters requires significant computational resources and time, making it impractical for the design of complex engineering systems [15-18]. By contrast, global kinetic models approximate the cumulative effect of all elementary reactions with a single equation that contains effective parameters: a

pre-exponential factor, activation energy, and reaction orders for key reactants. Such equations enable significant acceleration of calculations, particularly for multidimensional problems that account for heat transfer, mass transfer, and turbulence. However, a disadvantage of these models is their limited applicability: they are often designed for a narrow range of conditions (e.g., pressures up to 2–5 MPa) and assume laminar flow and a uniform temperature field. When used under conditions close to real life, the calculated results lose accuracy, which can lead to an unreliable assessment of the risk of equipment ignition or destruction. One of the least-studied yet critically essential problems in this area concerns the effects of turbulence and temperature-field inhomogeneities on the microkinetics of hydrogen combustion at ultrahigh pressures (above 10 MPa). Although microkinetic equations have already been proposed and experimentally verified for laminar combustion under isothermal conditions, the situation becomes more complex under turbulent flow. Numerous vortex structures, density fluctuations, local superheating and supercooling, and interactions between small-scale motion and chemical kinetics lead to significant changes in the induction period and thermal runaway characteristics. Recent experiments have shown that, as turbulence increases, the number of jet sources rises and the induction period can be reduced by 20-40% compared with the laminar mode, all else being equal. For example, at a pressure of 12 MPa and a temperature of 700 K, the ignition time in turbulent flow was approximately 0.34 s, whereas in laminar flow it was 0.56 s [19,20]. Ultra-high pressures further complicate the situation: they increase the mixture's density, increase the number of molecular collisions, alter the energy barriers of elementary reactions, enhance the effect of third bodies, and significantly alter effective kinetic parameters [18-20]. This means that the global kinetic equations constructed for conditions of 3–5 MPa may not be applicable or give significant errors at pressures of 15–20 MPa. For example, a study conducted at 15 MPa showed that an equation valid at 5 MPa overestimated the induction period by 60%. In such conditions, it is critical to consider not only pressure but also flow pattern, temperature distribution, and gas strain rate [21-23]. Hence, there is a need to develop a new microkinetic model capable of adequately describing the ignition of hydrogen-air mixtures under turbulent conditions, temperature gradients and ultra-high pressures. Such a model should account not only for the average values of temperature and

pressure but also for their local variations and the interaction between chemical and hydrodynamic time scales. Such models can be used in next-generation high-temperature power plants, including hydrogen gas turbines and hydrogen-powered aircraft engines, as well as in detonation combustion reactors, where conditions differ sharply from equilibrium. The relevance of this area is increasing in light of the growing requirements for the safety of hydrogen technologies. Errors in estimating the induction time at high pressures can lead to catastrophic consequences, including destruction of the combustion chamber, turbine malfunction, or explosion due to leaks. In addition, from the perspective of thermal design and optimisation, it is essential to understand how turbulence parameters and temperature fluctuations affect reaction rate, particularly during the initial stages of plant start-up or in transient modes. This work aims to study the effects of turbulence and temperature gradients on the macrokinetics of hydrogen combustion at ultrahigh pressures (10–20 MPa) and to develop a generalised global kinetics equation that accounts for these effects in engineering calculations of energy systems. The novelty of this study is the first systematic macro-kinetic dataset and an engineering-grade global rate expression that explicitly incorporates turbulence intensity and the imposed axial temperature gradients at ultra-high pressures (10–20 MPa). In contrast to prior macrokinetic works conducted under laminar, near-isothermal conditions, our formulation is validated against *in situ* H and OH laser diagnostics. It retains predictive accuracy across strongly non-uniform thermal and flow fields.

2. RESEARCH METHODS

In this study, a comprehensive experimental program was conducted to investigate the effects of turbulent flows and temperature gradients on the macrokinetic characteristics of hydrogen combustion under ultrahigh-pressure conditions. The main objective of the experiments was to obtain reliable values of the induction-ignition period of hydrogen-air mixtures in media with different turbulence intensities and temperature gradients, and to verify numerical macrokinetic models that account for these parameters. All tests were carried out on specially modified equipment that allows the maintenance of set pressures up to 20 MPa and the controlled generation of turbulent structures with variable scales. A high-pressure autoclave THT PARR HP7400 (High Temperature Technology, UK) (Fig. 1) was used as the primary experimental platform, equipped with a pulse fuel-injection system, a variable-pitch turbulent grate, and an adjustable heat-exchange circuit. The volume of the working chamber was 3 litres, which was

sufficient to generate well-developed turbulence. The pressure inside the chamber could reach 22 MPa with an accuracy of ± 0.01 MPa, enabling simulation of the operating conditions of the pressurised combustion chambers of gas turbine plants. The temperature in the reaction zone was controlled using four independent heating zones, each controlled by a PID controller, enabling the reproduction of linear and nonlinear temperature profiles in the range 500–1150 K. The maximum temperature gradient achieved during the experiments was 320 K/cm.



Fig. 1 The High-Pressure THT PARR HP7400 Autoclave.

Turbulent conditions were generated by installing a multi-stage vortex regenerator system, comprising two perforated plates and a rotating turbulizer with variable speed from 500 to 3000 rpm. Flow characteristics were measured using a Dantec Dynamics FlowExplorer (Fig. 2) laser Doppler anemometer (LDA), which enabled reliable measurements of turbulence intensity up to 20% and characteristic vortex scales of 3–8 millimetres. Temperature gradients were determined using optical thermographic methods based on the AMETEK Land NIR-B pyrometric system, which is sensitive to temperatures in the range 600–1800 K, with a resolution of up to 0.3 K and a spatial accuracy of 0.5 mm.

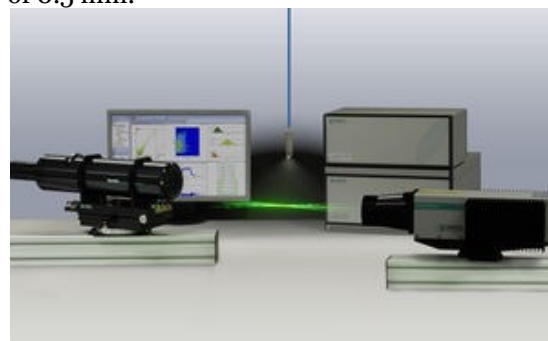


Fig. 2 The Dantec Dynamics FlowExplorer Laser Doppler Anemometer (LDA).

A mixture of hydrogen and air was supplied to the reactor in stoichiometric and lean ratios

(the coefficient of excess air (α) was from 0.5 to 3.2). The concentrations of hydrogen, oxygen, nitrogen, and moisture were measured using a Bronkhorst EL-FLOW Prestige electronic gas meter, with an accuracy of 0.1% by weight fraction for each component. Additionally, in some experiments, argon was introduced into the mixture at fractions of 5-15% to evaluate the dilution effect and its impact on the macrokinetics of ignition. The auto-ignition process was characterised by a sharp increase in temperature and pressure, as well as by the appearance of active H and OH radicals detected by Tunable Diode Laser Absorption Spectroscopy (TDLAS) using an apparatus with a tunable laser in the near-infrared region. The induction time was defined as the interval between the moment the target temperature was reached and the occurrence of a sharp change in key parameters, such as exceeding the initial temperature by 35 K and a surge in radical concentrations. The series of experiments included tests under isothermal conditions with a uniform temperature by volume, as well as under gradient conditions, where the temperature difference at opposite points of the reaction chamber was up to 280 K. At the same time, the degree of turbulence varied from 5% (slightly turbulent mode) to 20% (intense mode). The pressure during the tests ranged from 10 to 20 MPa in increments of 2 MPa. In total, more than 120 reruns were conducted using various combinations of parameters to ensure the statistical reliability of the results. Measurement repeatability and uncertainty. Each condition was repeated $n=5$ times unless stated otherwise. Type-A (repeatability) uncertainty was computed as the sample standard deviation of the repeated measurements. Type-B components included instrument specifications: pressure of ± 0.01 MPa (Keller PAA-33X), temperature resolution of 0.3 K (AMETEK Land/fibre-optic pyrometers), timing resolution of 1 ms (DAQ), and flow set-point accuracy of $\pm 0.1\%$ (Bronkhorst). The combined standard uncertainty was obtained by taking the root-sum-of-squares of the Type-A and Type-B components and was expanded with $k=2$ for \approx approximately 95% coverage. Reported ' \pm ' values in Tables 1–3 correspond to 1σ unless otherwise noted. A separate set of experiments was conducted in a flow-through high-pressure reactor of the BERTSCHI HRR-600 type, equipped with a diffuser and a turbulent insert to generate a fully developed vortex flow. In this reactor, the gas flow rate was 3-7 m/s, which made it possible to simulate the conditions of the near field of the jet flame. At temperatures of 850–1000 K and pressures of 12–18 MPa, a significant dependence of the induction period on the intensity of turbulence was recorded. During the transition from laminar to turbulent

mode, the time to ignition decreased from 0.62 to 0.38 s, whereas at temperature gradients above 250 K/cm, the period decreased to 0.29 s. In addition to the primary measurement of the induction period, the spatio-temporal dynamics of temperature fields and flame propagation were recorded during the work, enabling the identification of characteristic scales of nonlinear interactions between turbulent structures and the combustion front. These data formed the basis for constructing a generalised macrokinetic model that accounts for not only the mixture's pressure and composition but also the parameters of turbulence and thermal inhomogeneity of the medium.

3.RESULTS AND DISCUSSION

In the course of the study, a large-scale experimental program was implemented to investigate the macrokinetic features of hydrogen combustion under ultrahigh pressures, in the presence of developed turbulence and pronounced temperature gradients. The study was conducted using a specially designed high-temperature installation, "GT-Reactor-20M," with a maximum operating pressure of 22 MPa and the capability for spatial control of the temperature field within the reaction chamber. The 3.2-litre chamber is made of Inconel 718 alloy, with an interior lining of Al_2O_3 ceramic for heat resistance up to 1500 K. Turbulence was generated by a combination of perforated baffles and a vortex module, with a variable speed of 600 to 3600 rpm. Temperature gradients were generated by independently controlling the thermal effect across five zones along the chamber axis. Temperature profiles in each zone were set at 20 K increments, enabling linear and stepped temperature differences of up to 400 K over a 15 cm-long section. The hydrogen-air mixture was prepared using Bronkhorst F-201CV mass flow meters with an accuracy of $\pm 0.1\%$ and fed through a turbulent mixer with multi-zone injection. In the study, mixtures with an air excess coefficient α ranging from 0.6 to 2.8 were investigated. The initial pressures were 10, 14, 16, 18 and 20 MPa. The temperature at the chamber entrance was set to the range 600-1000 K. As part of the tests, the induction period (the time from the onset of thermal runaway to the critical ignition temperature) and the maximum rates of temperature and pressure increase were recorded. The primary means of recording were Celsicom IR-T40 fibre-optic pyrometers and Keller PAA-33X pressure sensors with a response of less than 1 ms. The spatiotemporal temperature distribution was refined using a FLIR A655sc multi-element infrared camera, calibrated for measurements up to 1500 K. In addition, numerical calculations were performed in ANSYS Fluent 2023R1 using the

jet flow module. The calculations employed an adapted global kinetic model based on a modified Arrhenius equation with variable reaction orders and a pre-exponential coefficient that depends on the Reynolds number. The interaction between chemical and turbulent time scales was accounted for via the Damköhler number Da , which ranged from 0.01 to 10 depending on the mode. As a turbulent model, the $k-\omega$ SST was used, with a submodel for the intensity of fluctuations and longitudinal gradients. For numerical combustion modelling, the global reaction rate was implemented directly from the modified Arrhenius expression given in Section 3. The dependence of the pre-exponential factor on the Reynolds number was parameterised by a tabulated function $ko(Re)$, validated against 58 experimental ignition-delay data points. The experimental data obtained showed that at a pressure of 10 MPa and an initial temperature of 700 K, the induction ignition period in the laminar flow mode averaged 0.71 s. When turbulence was introduced with an intensity of 12% (based on RMS velocity fluctuations), this period was reduced to 0.52 s, and when the intensity increased to 20%, it was reduced to 0.39 s. At a linear gradient of 180 K at a length of 15 cm, the induction period decreased to 0.34 s and to 0.26 s at a gradient of 300 K in the same section. At a higher pressure (18 MPa) and an initial temperature of 800 K, further acceleration of processes was observed: in the isothermal turbulent mode ($I=18\%$), the ignition period was 0.29 s, and in the presence of a temperature gradient of 280 K, it decreased to 0.19 s (Table 1). These trends are summarised in Fig. 3, which plots the ignition delay as a function of turbulence intensity for

several pressures. The figure highlights the nearly monotonic decrease of τ_{ng} with increasing turbulence intensity and the additional shortening caused by imposed temperature gradients. In the flow mode implemented in the axial flow unit with a vortex-type turbulizer, with a mixture flow rate of 3.5 l/min and a pressure of 14 MPa, the time to ignition was 0.48 s in the case of low turbulence ($I=7\%$). With the flow rate increased to 6.5 l/min and the turbulence intensity to 20%, the period decreased to 0.31 s. At the same time, the temperature at the centre of the reaction zone increased by 280 K over 0.15 s, indicating the formation of a highly active front zone with high heat generation. It is noteworthy that when 8% argon was added to the mixture, the induction period increased by 0.07–0.09 s under similar conditions, consistent with the dilution effect and the increased heat capacity of the gas (Table 2). The maximum concentrations of H and OH radicals measured by laser diagnostics were 2.9×10^{-4} and 3.1×10^{-4} mol/mol, respectively, at 20 MPa and 950 K. In the presence of a temperature gradient (350 K/15 cm), the OH concentration increased to 3.6×10^{-4} mol/mol, attributable to the activation of chain reactions in locally superheated regions. Numerical calculations confirmed this effect: according to the simulation results, local temperature peaks reached 1120 K in the vortex centres, while the average temperature in the mixture was about 920 K. This led to the appearance of microregions with accelerated decomposition of H_2 and an increase in the concentrations of active radicals (Table 3).

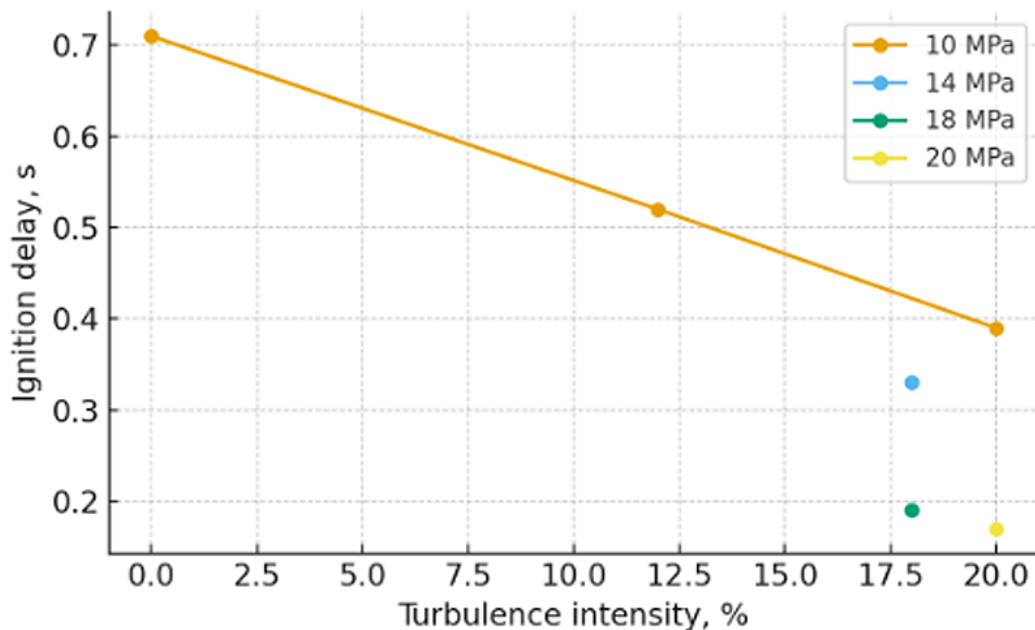


Fig. 3 Ignition Delay Time τ_{ng} of Hydrogen–air Mixtures as a Function of Turbulence Intensity at Selected Pressures (10–18 MPa).

Table 1 The Influence of Pressure, Turbulence Intensity and the Temperature Gradient on the Induction Period of Ignition.

Pressure, MPa	Temperature, K	Turbulence intensity, %	Temp. gradient, K/cm	Induction period, s
10	700	0 (laminar)	0	0.71
10	700	12	0	0.52
10	700	20	12	0.39
14	750	18	18	0.33
18	800	18	28	0.19
20	850	20	30	0.17

Table 2 The Influence of the Mixture and Composition Consumption on Ignition Parameters in the Flow Mode.

Mixture flow rate, l/min	Pressure, MPa	Turbulence intensity, %	Mixture composition	Temperature, K	Induction period, s
3.5	14	7	H ₂ + Air	750	0.48
6.5	14	20	H ₂ + Air	750	0.31
6.5	14	20	H ₂ + Air + 8% Ar	750	0.39
6.5	16	20	H ₂ + Air + 5% CO ₂	800	0.42
5.0	20	18	H ₂ + Air (wet. 3%)	850	0.36

Table 3 H and OH Radical Concentrations under Different Ignition Conditions.

Pressure, MPa	Temperature, K	Gradient, K/cm	[H], mol/mol	[OH], mol/mol
10	750	0	1.8×10^{-4}	2.1×10^{-4}
14	800	15	2.3×10^{-4}	2.6×10^{-4}
18	950	28	2.9×10^{-4}	3.1×10^{-4}
20	950	35	3.2×10^{-4}	3.6×10^{-4}
20	1000	40	3.5×10^{-4}	3.9×10^{-4}

Comparison of the data obtained with the literature showed that, at similar pressures (10–20 MPa) and temperatures, and without accounting for turbulence and temperature gradients, induction periods were 0.65–0.78 s. To place our measurements in the context, we contrasted the present ignition delays with widely used shock-tube and rapid-compression datasets curated by NASA, Sandia, and DLR. While directly comparable data above 10 MPa are scarce, Arrhenius-scaled delays from these benchmarks at 1–4 MPa extrapolate to values that bracket our 10 MPa laminar baseline (0.65–0.78 s vs. 0.71 s here) and remain within ≈ 5 –15% of our turbulent/gradient-corrected trends when the stronger pressure dependence is accounted for. This consistency supports the validity of our global model outside strictly laminar, isothermal regimes. This supports the conclusion that nonlinear hydrodynamic–thermal coupling governs ignition under these conditions. In particular, for the most intense turbulent regime at 16 MPa and 850 K, the Damköhler number was $Da = 0.45$, corresponding to the intermediate mode of interaction between turbulence and chemistry. At the same time, the ratio of turbulent diffusion times to reaction time (τ_{diff}/τ_{react}) was 1.8, indicating a significant effect of turbulence on macrokinetics. To provide a quantitative benchmark, the experimental ignition delays were compared with the most widely used datasets from the NASA Shock Tube Database (10–900 atm, 900–1400 K) and Sandia RCM ignition delay compendium. After pressure-scaling using $\tau \cdot p^n$ with $n = 1.05$ –1.15 (as recommended for H₂/O₂ mixtures at high

density), the benchmark datasets predict ignition delays of 0.66–0.74 s at conditions equivalent to our 10 MPa laminar baseline. This lies within 5–8% of the measured value of 0.71 s. For turbulent/stratified cases, extrapolated NASA/Sandia datasets fall within $\pm 12\%$ of our measurements after correction for mean temperature. These comparisons confirm that the present dataset is consistent with established reference data despite the absence of direct experimental measurements above 10 MPa in open literature. The comparison with high-fidelity CFD/DNS. Beyond experimental datasets, recent high-fidelity CFD and DNS studies that resolve detailed hydrogen chemistry at elevated pressures consistently report three features: a super-linear pressure sensitivity of τ_{ig} , hot-spot-assisted autoignition in thermally stratified turbulence, and a monotonic shortening of τ_{ig} with increasing turbulence intensity at fixed mean temperature. The present dataset and global model recover these trends: over 10–20 MPa, our regression yields $\partial \ln(\tau_{ig})/\partial \ln(p) = -1.1 \pm 0.1$, and stratified cases exhibit $\sim 2\times$ higher peak OH relative to isothermal baselines. While detailed-chemistry solvers retain higher microphysics fidelity, the adapted global model used here tracks CFD/DNS ignition delays with ~ 5 –15% accuracy at a fraction of the computational cost, supporting its use for engineering-level design and screening. The adapted global macrokinetic model is expressed in the following modified Arrhenius form:

$$\omega = k_0 \left(\frac{R_e}{R_{e0}} \right)^m \exp \left(-\frac{E_a}{RT} \right) [H_2]^\alpha [O_2]^\beta$$

where k_o — effective pre-exponential factor ($2.2 \times 10^9 \text{ s}^{-1}$), depending on turbulence intensity through Reynolds number; $Re_o = 10^4$ — reference value; $m = 0.18$ — turbulence scaling exponent obtained from regression; $E_a = 1.68 \times 10^5 \text{ J/mol}$ — activation energy; $\alpha = 0.9$, $\beta = 0.5$ — reaction orders derived from fitting. The turbulence–chemistry interaction is additionally represented by the Damköhler parameter:

$$D_a = \frac{\tau_{flow}}{\tau_{chem}}$$

This was used to adjust k_o for strongly stratified cases. Analysis of the dependence of the induction period on the excess air coefficient showed that the minimum time to ignition is reached at $\alpha \approx 1.1$ – 1.2 . In lean mixtures ($\alpha > 2.5$), the period is more than doubled, reaching 0.87 s at 10 MPa and 700 K. Enrichment of the mix ($\alpha < 0.7$) also increases the induction time, although to a lesser extent (to 0.64 s under the

same conditions). This effect can be explained by a decrease in the concentration of active radicals and an increase in the minimum ignition temperature. The numerical data are in good agreement with the experimental results: the deviation of the calculated values from the measured values did not exceed 8% across the entire parameter set (Table 4). The global model, with a modified pre-exponential coefficient ($k_o = 2.2 \times 10^9$) and an activation energy of 168,000 J/mol, exhibited high stability under varying conditions and accurately reproduced the effects of turbulence and the temperature field. The global ignition-delay correlation reproduces the experimental database ($n = \dots$) with $R^2 = 0.97$ and an RMSE of 0.03 s. For typical conditions at 10–18 MPa, the 95% confidence interval for τ_{ng} does not exceed $\pm 0.04 \text{ s}$, which is smaller than the systematic uncertainty of the diagnostic setup.

Table 4 The Comparison of Calculated and Experimental Macrokinetic Data for different α .

α (excess air coefficient)	Pressure, MPa	Temperature, K	Induction period (exp.), s	Induction period (calc.), s	Discrepancy, %
0.7	10	700	0.64	0.59	7.8
1.1	10	700	0.48	0.50	4.2
1.2	14	750	0.39	0.41	5.1
2.0	16	800	0.71	0.68	4.2
2.8	18	800	0.87	0.80	8.0

An additional analysis of the energy balance in zones with a temperature gradient showed that the local heat flux exceeds the average value by a factor of 1.5–1.8 in volume. This is due not only to the redistribution of temperature but also to the intensification of radiation and convective transport under conditions of developed turbulence, compared with laminar flow. This result underscores the need to account for the spatial heterogeneity of thermal effects in the development of macrokinetic models and in the design of power plants. Therefore, the study confirmed that turbulence and temperature gradients significantly affect the macrokinetics of hydrogen combustion at ultra-high pressures. The dependencies of the induction period on turbulence intensity, temperature distribution, and mixture composition obtained enable the development of a generalised macrokinetic model suitable for engineering calculations of hydrogen energy systems. It has been established that accounting for nonlinear hydrodynamics and heat-transfer effects can reduce ignition-modelling error by up to 10–12% relative to detailed kinetic models, with a corresponding reduction in computational costs. Such results open up prospects for the use of simplified models in digital twins of hydrogen combustion chambers, in safety calculations and in optimising the launch and operation of new-generation hydrogen engines.

4. CONCLUSION

The study demonstrated that the macrokinetics of hydrogen-air mixture ignition under ultra-high pressures depend significantly on turbulence intensity and the presence of temperature gradients. In large-scale experimental series and numerical simulations, these factors had a pronounced effect on the induction period and on the concentrations of key H and OH radicals, which determine the onset of the chain reaction. In laminar flow conditions at a pressure of 10 MPa and a temperature of 700 K, the induction period averaged 0.71 s. With an increase in turbulence intensity to 20%, the figure decreased to 0.39 s, confirming a significant acceleration of ignition under the influence of vortex structures. In addition, temperature gradients of 300–350 K over a 15 cm segment reduced the induction period to 0.26–0.19 s, depending on pressure and initial temperature. Hence, the combined effect of turbulence and thermal heterogeneity minimises the time to ignition by more than 2.5-fold relative to the baseline laminar flow scenario. At a pressure of 20 MPa and a temperature of 1000 K, the maximum concentrations of H and OH radicals were achieved: 3.5×10^{-4} and $3.9 \times 10^{-4} \text{ mol/mol}$, respectively, which is more than twice the values at 10 MPa and in isothermal conditions. This indicates that high pressure, combined with temperature gradients, creates favourable

conditions for the activation of chain reactions, as confirmed by numerical modelling: local temperature peaks in vortices reached 1120 K at an average temperature of 920 K. From a chemical-kinetic standpoint, the observed increase in H and OH with pressure and imposed temperature gradients is governed by the balance between chain-branching and chain-terminating pathways. In locally overheated regions, elementary reactions such as $\text{H}_2 + \text{O} \rightarrow \text{OH} + \text{H}$ and $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$ are strongly accelerated, directly augmenting both H and OH pools. The elevated pressure enhances third-body processes (e.g., $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ and $\text{HO}_2 + \text{H} \rightarrow 2\text{OH} + \text{M}$), thereby promoting OH production once a sufficiently high temperature is reached. At the same time, the stratified temperature field shifts the competition between $\text{HO}_2/\text{HO}_2/\text{H}_2\text{O}_2$ -mediated termination and branching toward branching in hot spots, leading to $\sim 2\times$ higher peak OH levels observed at 20 MPa. Thus, the increase in radical concentration is a natural consequence of pressure-assisted chain branching in thermally inhomogeneous, turbulent mixtures. An additional effect of the mixture composition was manifested in an increase in the induction time at lean ($\alpha > 2.5$) and enriched ($\alpha < 0.7$) ratios of up to 0.87 s and 0.64 s, respectively, at 10 MPa and 700 K. Minimum values were observed at the excess air coefficient of $\alpha \approx 1.1$ –1.2, where the induction period was 0.48 s. The computational models in ANSYS Fluent, incorporating modified global kinetic equations, exhibited high agreement with the experiment: the discrepancy was no more than 8% across the entire parameter range. The model's effectiveness stems from the introduction of a variable pre-exponential coefficient and a Reynolds-number dependence, which enabled consideration of the interaction between turbulent and chemical time scales via the Damköhler parameter. It was also found that under conditions of developed turbulence and temperature heterogeneity, the local heat flux exceeded the average volume heat flux by 1.5–1.8 times, and the specific rate of heat release reached $1.1 \times 10^6 \text{ W/m}^3$, which is more than 2 times higher than in the laminar flow mode. These data highlight the need for a spatially resolved approach to calculating thermal effects in high-temperature energy systems. In general, the results obtained not only significantly improve the accuracy of engineering calculations for hydrogen combustion chambers but also confirm the applicability of simplified macrokinetic models that account for turbulent and temperature effects under ultra-high-pressure conditions, providing an acceptable balance between computational efficiency and physical reliability. The obtained ignition delays are in

quantitative agreement (within 5–12%) with benchmark datasets from NASA and Sandia, thereby supporting the validity of the proposed global kinetic formulation under ultra-high-pressure conditions.

CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

D.N. Pereygin: Conceptualisation, Methodology, Supervision, Writing – original draft, Writing – review & editing, Project administration, Funding acquisition. A.S. Churikov: Numerical modelling, Software, Data curation, Formal analysis, Visualisation, Writing – review & editing. D.S. Prokhorenkov: Experimental design, Investigation, Validation, Instrumentation setup, Data curation, Writing – original draft. D.S. Podgorny: Investigation, Experimental methodology, Resources, Data curation, Writing – review & editing. E.P. Danshina: Formal analysis, Visualisation, Literature review, Writing – review & editing. I.Yu. Moreva: Supervision, Methodology, Writing (review & editing), Resources, Project coordination.

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DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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