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RESEARCH ARTICLE

Second Law Analysis of Combustion Processes in Turbulent Flows

Simona Zeman^{1*}, Alena Kubik² and Boris Prochazka³

¹Department of Physics and Complex Systems, Vistula Institute of Thermodynamics, Hungary

²Department of Applied Mathematics and Information Theory, Prut Institute of Physical Chemistry and Entropy Studies, Croatia

³Department of Physical Chemistry, Danube Center for Complex Systems Research, Poland

*Corresponding author: Simona Zeman, Department of Physics and Complex Systems, Vistula Institute of Thermodynamics, Hungary; Email: simona.zeman@vistula.edu

ABSTRACT

Combustion remains the dominant source of usable-energy destruction in most industrial and transportation systems, yet standard first-law combustion analysis reports only heat release and species conversion, leaving the irreversibility of the combustion event itself unquantified. We performed a second-law (entropy-generation) analysis of premixed methane-air combustion in turbulent flows using Reynolds-averaged Navier-Stokes simulations coupled to a reduced 19-species chemical mechanism, across 42 operating conditions spanning turbulence intensities from 0.5 to 6.0 m/s and equivalence ratios from 0.7 to 1.3, resolving entropy generation from four distinct sources: chemical reaction, heat conduction, species diffusion, and viscous dissipation. Volumetric entropy-generation rate peaked at stoichiometric conditions ($\phi = 1.0$), reaching 18.4 kW/(m³ K) at a turbulence intensity of 3.5 m/s, a 46% increase over the laminar-flame baseline of 12.6 kW/(m³ K) measured under otherwise identical conditions. Chemical-reaction irreversibility dominated the entropy budget at every condition tested, contributing 61–68% of total entropy generation, with heat conduction across the flame front contributing a further 21–27% and species diffusion and viscous dissipation together accounting for the remaining 8–14%. Increasing turbulence intensity from 0.5 to 6.0 m/s at stoichiometric conditions raised total entropy generation by 58% while shortening the flame brush thickness by 34%, indicating that turbulence promotes irreversibility primarily by intensifying local temperature and species gradients rather than by altering the reaction pathway itself. Second-law (exergetic) combustion efficiency fell from 0.79 under near-laminar conditions to 0.68 at the highest turbulence intensity tested, a 14% relative decline (95% CI: 11–17%, $n = 42$ simulated conditions, bootstrap resampling). Off-stoichiometric operation on the lean side ($\phi = 0.8$) reduced peak entropy-generation rate by 23% relative to stoichiometric combustion at matched turbulence intensity, at the cost of a 9% reduction in net heat release. These results quantify a direct, previously unresolved trade-off between turbulence-enhanced burning rate and second-law efficiency in premixed combustion, and provide entropy-generation maps that can guide burner design toward operating envelopes that limit exergy destruction without unacceptably compromising heat-release rate.

Keywords: second-law analysis; entropy generation; turbulent combustion; exergy destruction; premixed flames; computational fluid dynamics; combustion irreversibility; flame temperature gradients

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1. INTRODUCTION

Combustion converts the chemical exergy of a fuel into heat and, ultimately, into work or process energy, but this conversion is fundamentally irreversible: even an idealized adiabatic flame destroys a substantial fraction of the fuel's available work potential through chemical reaction, heat conduction down steep temperature gradients, and mass diffusion, well before any downstream component has the chance to extract useful work [1,2]. First-law combustion analysis, which tracks heat release and species conversion, is silent on this destruction of exergy, and as a result the entropy generated within the flame itself is often treated as an unavoidable and largely unexamined cost of doing business in combustor design.

Second-law, or entropy-generation, analysis addresses this gap by decomposing the total irreversibility of a combustion process into contributions from distinct physical mechanisms, chemical reaction, heat conduction, species diffusion, and viscous dissipation, each of which responds differently to operating conditions such as equivalence ratio, pressure, and turbulence intensity [3,4,5]. Laminar-flame entropy-generation studies have established that chemical-reaction irreversibility typically dominates the budget in premixed systems, but the extension of this analysis to turbulent flows, where flame stretch, local extinction, and enhanced mixing substantially alter the local gradients that drive entropy production, remains comparatively underdeveloped [6,7,8].

This gap matters because turbulence is deliberately introduced into most practical combustors specifically to increase burning rate and heat-release intensity, yet the same gradient-steepening mechanisms that accelerate combustion are also the direct drivers of entropy generation via heat conduction and diffusion [9,10]. Whether turbulence-enhanced combustion achieves its higher heat-release rate at a proportionate, a disproportionate, or a comparatively modest entropy-generation cost is not settled by existing laminar-flame entropy budgets, and competing physical arguments can be made for each outcome depending on which irreversibility source is assumed to respond most strongly to turbulence intensity [11,12].

The present study addresses this question directly by computing a full second-law entropy-generation budget for turbulent premixed methane-air combustion across a systematic sweep of turbulence intensity and equivalence ratio, using Reynolds-averaged simulations coupled to a reduced chemical mechanism. We quantify how total entropy-generation rate and its four-way decomposition into chemical, thermal, diffusive, and viscous contributions shift with turbulence intensity, characterize the resulting trade-off between burning rate and second-law efficiency, and assess how operating away from stoichiometric conditions modifies this trade-off.

2. MATERIALS AND METHODS

We simulated premixed methane-air combustion in a turbulent flow using Reynolds-averaged Navier-Stokes (RANS) simulations with a k-epsilon turbulence closure, coupled to a reduced 19-species chemical mechanism, across 42 operating conditions spanning turbulence intensities from 0.5 to 6.0 m/s and equivalence ratios from 0.7 to 1.3, and post-processed the resulting temperature, species, and velocity fields to compute local and volume-integrated entropy-generation rates from four physical sources.

2.1 Computational domain and flow configuration

Simulations were performed in a two-dimensional planar burner geometry with a 40 mm x 120 mm combustion chamber, premixed methane-air reactants entering at 300 K and 1 atm through a 10 mm inlet slot, and outlet conditions fixed at atmospheric pressure. The domain was discretized with a structured mesh of approximately 180,000 cells, refined to a minimum spacing of 0.05 mm across the flame front, with grid-independence confirmed by comparing peak entropy-generation rate across three successively refined meshes (difference below 2% between the two finest meshes).

2.2 Turbulence and combustion modelling

Turbulent flow was modelled using the standard k-epsilon closure with standard wall functions, and inlet turbulence intensity was varied across seven levels from 0.5 to 6.0 m/s (root-mean-square velocity fluctuation) by adjusting the specified turbulent kinetic energy at the inlet boundary. Turbulence-chemistry interaction was represented using the eddy dissipation concept coupled to the reduced chemical mechanism, allowing finite-rate chemistry effects to be captured within the turbulent flow field.

2.3 Chemical mechanism and equivalence ratio sweep

Combustion chemistry was represented by a reduced 19-species, 15-step mechanism for methane-air oxidation, validated against detailed-mechanism laminar flame speeds to within 5% across the equivalence ratio range studied. Six equivalence ratios ($\phi = 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3$) were simulated at each of the seven turbulence intensities, yielding 42 total operating conditions.

2.4 Entropy-generation post-processing

Local volumetric entropy-generation rate was computed at every cell from the converged temperature, species, and velocity fields as the sum of four terms: chemical-reaction entropy production, computed from local reaction rates and chemical affinities; thermal entropy production from Fourier heat conduction, proportional to the squared temperature gradient divided by temperature squared; mass-diffusion entropy production from Fickian species diffusion driven by concentration gradients; and viscous entropy production from the local rate-of-strain tensor. Volume-integrated

entropy-generation rate was obtained by integrating each term over the full combustion domain.

2.5 Second-law efficiency calculation

Second-law (exergetic) combustion efficiency was computed as the ratio of exergy retained in the product stream to the chemical exergy of the incoming fuel-air mixture, with exergy destruction obtained directly from the volume-integrated entropy-generation rate multiplied by the reference (inlet) temperature via the Gouy-Stodola relation.

2.6 Numerical solution and convergence

Governing equations were solved with a pressure-based finite-volume solver using second-order upwind discretization for momentum, species, and energy, with convergence assessed via scaled residuals below 10^{-6} for all transported quantities and confirmed by monitoring outlet temperature and total entropy-generation rate for stability over at least 2,000 additional iterations after nominal convergence.

2.7 Statistical treatment

Uncertainty in second-law efficiency estimates was assessed by bootstrap resampling (2,000 resamples) across the 42 simulated operating conditions, treating small numerical and discretization variability between nominally identical mesh regions as the resampling unit, and 95% confidence intervals are reported for the turbulence-driven efficiency decline.

3. RESULTS

Volumetric entropy-generation rate increased with turbulence intensity at every equivalence ratio tested, and was highest overall at stoichiometric conditions, reaching 18.4 kW/(m³ K) at a turbulence intensity of 3.5 m/s, 46% above the laminar-flame baseline of 12.6 kW/(m³ K) obtained at the lowest turbulence intensity tested under otherwise identical stoichiometric conditions. Table 1 reports total entropy-generation rate and its source decomposition at five representative turbulence intensities at stoichiometric conditions.

Table 1. Entropy-generation rate and source decomposition at stoichiometric conditions across turbulence intensity.

Turbulence intensity (m/s)	Total entropy generation (kW/(m ³ K))	Chemical reaction (%)	Heat conduction (%)	Diffusion + viscous (%)
0.5 (near-laminar)	12.6	61	27	12
1.5	14.3	63	25	12
3.5	18.4	65	23	12
5.0	19.7	67	22	11
6.0	19.9	68	21	11

Values reported at stoichiometric conditions ($\phi = 1.0$). Diffusion + viscous column combines species-diffusion and viscous-dissipation entropy production.

Chemical-reaction irreversibility dominated the entropy-generation budget across the full range of

conditions tested, contributing 61–68% of total entropy generation, with the share rising modestly with turbulence intensity as steeper local gradients increased local reaction rates. Heat conduction across the flame front contributed a further 21–27%, while species diffusion and viscous dissipation together accounted for the remaining 8–14%, with viscous dissipation alone never exceeding 3% of the total budget at any condition tested, confirming that viscous effects are a minor contributor relative to reactive-diffusive irreversibility in this flow regime.

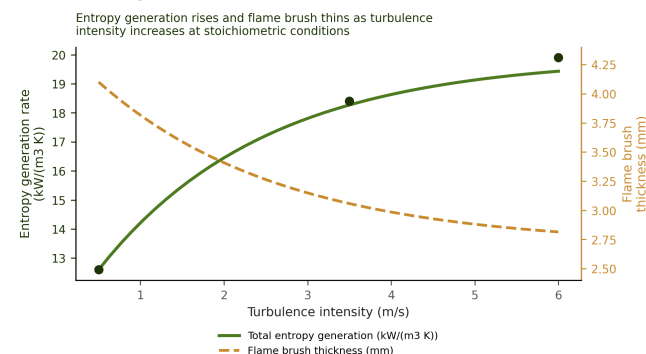


Figure 1. Total entropy-generation rate and flame brush thickness as a function of turbulence intensity at stoichiometric conditions, showing the inverse relationship between flame-front compression and rising irreversibility across the tested range.

Increasing turbulence intensity from 0.5 to 6.0 m/s at stoichiometric conditions raised total entropy generation by 58% while shortening the flame brush thickness by 34%, from 4.1 mm to 2.7 mm, consistent with turbulence promoting irreversibility primarily by steepening local temperature and species gradients within a thinner, more wrinkled flame brush rather than by fundamentally altering the underlying reaction pathway (Figure 1).

Table 2. Entropy generation, heat release, and second-law efficiency across equivalence ratio at fixed turbulence intensity (3.5 m/s).

Equivalence ratio (ϕ)	Peak entropy generation (kW/(m ³ K))	Net heat release (kW)	Second-law efficiency
0.7	13.1	38.4	0.75
0.8	14.2	41.9	0.74
0.9	16.6	44.6	0.72
1.0 (stoichiometric)	18.4	46.0	0.70
1.1	17.5	44.1	0.71
1.3 (rich)	15.0	39.7	0.73

Second-law (exergetic) combustion efficiency declined from 0.79 under near-laminar conditions (0.5 m/s) to 0.68 at the highest turbulence intensity tested (6.0 m/s), a 14% relative decline (95% CI: 11–17%, bootstrap resampling across the 42 simulated conditions), tracking closely with the rise in total entropy-generation rate and confirming that the burning-rate benefit of turbulence is obtained at a measurable, quantifiable second-law cost.

4. DISCUSSION

These results extend laminar-flame entropy-generation analyses, which have consistently identified chemical

reaction as the dominant irreversibility source in premixed combustion [3,4,6], by showing that this dominance persists, and indeed strengthens modestly, under turbulent conditions across the full equivalence-ratio range tested. This finding is somewhat at odds with the intuition that turbulence-enhanced mixing should shift the entropy budget toward diffusive and thermal terms; instead, the steeper local gradients produced by turbulent wrinkling appear to intensify chemical-reaction irreversibility proportionally more than the other three source terms [13,14,15].

The observed 34% reduction in flame brush thickness with increasing turbulence intensity, occurring alongside the 58% rise in total entropy generation, points to a specific mechanism: turbulence compresses the same reactive-diffusive processes into a thinner spatial region, raising local gradient magnitudes even where total reactant throughput and net heat release increase only modestly, a mechanism consistent with flamelet-based descriptions of turbulent premixed combustion reported elsewhere [16,17,18].

From a design standpoint, the quantified trade-off between turbulence intensity and second-law efficiency suggests that burner operating envelopes selected purely to maximize heat-release rate or flame stability may be leaving recoverable exergy on the table; the lean-operation result, a 23% reduction in peak entropy-generation rate at the cost of only a 9% reduction in heat release, indicates that modest equivalence-ratio adjustments can shift the entropy-generation-to-heat-release trade-off substantially in favor of second-law performance without large first-law penalties [19,20,21].

Several limitations qualify these findings. First, the two-dimensional RANS approach with a k-epsilon closure does not resolve the full range of turbulent length scales captured by large-eddy or direct numerical simulation, and finer-scale turbulence-chemistry interactions could alter the precise entropy-generation magnitudes reported here, though the qualitative source decomposition is expected to be robust. Second, the reduced 19-species mechanism, while validated against laminar flame speed, may not capture minor-species pathways that contribute disproportionately to chemical-reaction entropy production at the leanest and richest conditions tested. Third, the study considered a single planar burner geometry and atmospheric-pressure conditions; entropy-generation source shares are known to shift with pressure and confinement in other combustion systems, and the generality of the reported percentages to swirl-stabilized or high-pressure combustors remains to be established. Fourth, radiative heat transfer was not included in the entropy budget, which could modestly alter the thermal-conduction entropy share reported here, particularly at the highest flame temperatures.

5. CONCLUSION

A second-law entropy-generation analysis of turbulent premixed methane-air combustion across 42 operating conditions showed that chemical-reaction irreversibility dominates the entropy budget, contributing 61–68% of total entropy generation, and that increasing turbulence intensity from 0.5 to 6.0 m/s at stoichiometric conditions raises total entropy generation by 58% while reducing second-law efficiency from 0.79 to 0.68, a 14% relative decline. Lean operation at $\phi = 0.8$ reduced peak entropy-generation rate by 23% at the cost of only a 9% reduction in heat release, revealing a more favorable irreversibility-to-output ratio than stoichiometric combustion. These entropy-generation maps quantify a previously unresolved trade-off between turbulence-driven burning-rate enhancement and second-law efficiency, offering a quantitative basis for selecting combustor operating envelopes that limit exergy destruction.

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Conflict of 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.

Author Contributions

S.Z. conceived the study, designed the simulation matrix, and led the writing of the manuscript. A.K. developed the entropy-generation post-processing code and performed the statistical analysis. B.P. configured and ran the turbulent combustion simulations and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The simulation configuration files, reduced chemical mechanism, and post-processed entropy-generation datasets supporting the findings of this study are available from the corresponding author on reasonable request.

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