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RESEARCH ARTICLE

Thermodynamic Analysis of Irreversibility in Microfluidic Mixing Devices

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ABSTRACT

Microfluidic mixing devices must generate species-concentration uniformity within channel lengths of only a few millimeters, and doing so under laminar, low-Reynolds-number flow necessarily relies on chaotic advection structures that dissipate mechanical energy and generate entropy through both viscous friction and irreversible mass diffusion, yet the relative size of these two irreversibility sources across realistic operating conditions is not always reported quantitatively for a given mixer geometry. We performed a second-law (entropy generation minimization) analysis of a staggered-herringbone passive micromixer combining computational fluid dynamics with a scalar transport solver across 40 operating conditions spanning flow rates from 5 to 200 $\mu\text{L}/\text{min}$ (Reynolds number 0.02–0.9, Peclet number 1.2×10^3 – 4.8×10^4). Total volumetric entropy generation rate increased from $3.1 \times 10^{-3} \text{ W}/(\text{m}^3 \text{ K})$ at the lowest flow rate to $2.86 \text{ W}/(\text{m}^3 \text{ K})$ at the highest, a roughly 920-fold increase, with the balance between viscous and diffusive (concentration-gradient) contributions shifting systematically across this range: diffusive entropy generation dominated at low flow rate (81% of total at 5 $\mu\text{L}/\text{min}$) while viscous entropy generation dominated at high flow rate (76% of total at 200 $\mu\text{L}/\text{min}$), crossing over at an intermediate flow rate of approximately 42 $\mu\text{L}/\text{min}$. The mixing index, defined from the coefficient of variation of outlet concentration, improved from 0.61 at the lowest flow rate to 0.94 at 80 $\mu\text{L}/\text{min}$ but then plateaued, reaching only 0.96 at the highest flow rate tested, while total entropy generation over the same interval more than quadrupled, indicating strongly diminishing thermodynamic returns on mixing quality beyond roughly 80 $\mu\text{L}/\text{min}$. A dimensionless Bejan number, the ratio of diffusive to total entropy generation, decreased monotonically from 0.81 to 0.24 across the tested flow range ($R^2 = 0.97$ for a power-law fit against Peclet number), and a geometric parameter sweep varying herringbone groove depth by $\pm 25\%$ shifted the crossover flow rate by up to 18% while changing peak mixing index by less than 2 percentage points. These results identify an operating window, approximately 60–90 $\mu\text{L}/\text{min}$ for this geometry, in which near-complete mixing is achieved without incurring the steep entropy-generation penalty of substantially higher flow rates, providing a quantitative second-law basis for selecting operating conditions in passive microfluidic mixer design.

Keywords: microfluidic mixing; entropy generation minimization; viscous dissipation; herringbone micromixer; irreversibility; Peclet number; mixing index; second-law analysis

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1. INTRODUCTION

Passive microfluidic mixers achieve species mixing without moving parts by using channel geometry, most commonly grooved or herringbone surface patterns, to generate chaotic advection that stretches and folds fluid striations under otherwise strictly laminar, low-Reynolds-number flow [1,2]. Because diffusion alone is far too slow to homogenize concentration across typical microchannel widths within practical channel lengths, this induced chaotic advection is essential to achieving useful mixing performance in lab-on-a-chip, chemical synthesis, and diagnostic microfluidic applications [3,4].

Second-law (entropy generation minimization) analysis provides a thermodynamic lens for evaluating such mixers that complements purely kinematic mixing-index metrics, since both the viscous dissipation associated with driving flow through the channel and the irreversible diffusion of species down a concentration gradient generate entropy, and a device that mixes well only by paying a disproportionate viscous-dissipation penalty is not necessarily the most thermodynamically efficient design choice [5,6,7]. This framework, developed originally for heat-exchanger and thermal-system design, has been extended to microfluidic mass-transfer devices in a growing body of work, but studies quantifying how the viscous and diffusive entropy-generation contributions trade off against one another across a full practical flow-rate range for a specific, widely used mixer geometry remain comparatively limited [8,9,10].

This matters for design because mixing index alone does not indicate whether a given improvement in mixing quality is being purchased at a proportionate or disproportionate thermodynamic cost, and identifying the flow regime in which the two entropy-generation sources are comparable, and beyond which further flow-rate increases yield diminishing mixing returns for a steeply rising entropy cost, gives microfluidic device designers a quantitative operating window rather than a single optimum defined by mixing index alone [11,12,13].

The present study performs a combined computational fluid dynamics and scalar transport second-law analysis of a staggered-herringbone passive micromixer across a wide range of flow rates, decomposing total entropy generation into its viscous and diffusive components, identifying the flow rate at which the two contributions are equal, relating entropy generation to mixing index across the same flow-rate range to identify diminishing returns, and testing the sensitivity of these findings to herringbone groove depth.

2. MATERIALS AND METHODS

We performed coupled computational fluid dynamics and scalar transport simulations of a staggered-herringbone passive micromixer across 40 flow-rate operating conditions from 5 to 200 $\mu\text{L}/\text{min}$, computing local viscous and diffusive entropy generation rates,

integrating them to obtain total volumetric entropy generation, and comparing this thermodynamic metric against a directly computed mixing index.

2.1 Mixer geometry and computational domain

The simulated device was a staggered-herringbone micromixer with a main channel of 200 μm width and 70 μm depth, patterned with asymmetric herringbone grooves (30 μm groove depth, baseline) repeating every randomly ridge-cycled six-groove sequence over a 3 cm mixing length, following the geometry class widely used in prior chaotic-advection micromixer studies. The computational domain was discretized with an unstructured tetrahedral mesh refined to 8 μm near groove walls, totaling approximately 2.1 million elements, with mesh-independence confirmed by a doubling-refinement check showing less than 1.5% change in predicted mixing index.

2.2 Flow and scalar transport solver

Steady-state laminar flow was solved using a finite-volume Navier-Stokes solver for incompressible flow of an aqueous working fluid (density 998 kg/m^3 , viscosity $1.0 \times 10^{-3} \text{ Pa}\cdot\text{s}$), and a coupled scalar transport equation was solved for a passive tracer species with diffusivity $1.0 \times 10^{-9} \text{ m}^2/\text{s}$, introduced as two co-flowing streams at the channel inlet at equal flow rate and opposite unit/zero concentration.

2.3 Operating-condition sweep

Forty operating conditions were simulated with total inlet flow rate ranging from 5 to 200 $\mu\text{L}/\text{min}$, corresponding to Reynolds numbers from 0.02 to 0.9 and Peclet numbers from 1.2×10^3 to 4.8×10^4 , sampled with finer spacing at low and intermediate flow rates where the balance of entropy-generation sources was expected to shift most rapidly.

2.4 Entropy generation rate calculation

Local volumetric entropy generation rate was computed as the sum of a viscous dissipation term, derived from the local velocity-gradient tensor and fluid viscosity, and a diffusive (concentration-gradient) term, derived from the local concentration-gradient magnitude and species diffusivity following standard entropy generation minimization formalism; both terms were integrated over the full channel volume at each operating condition to obtain total, viscous, and diffusive volumetric entropy generation rates.

2.5 Mixing index calculation

Mixing index at the channel outlet was computed as 1 minus the coefficient of variation of the cross-sectional concentration profile, normalized so that a value of 1 corresponds to perfectly uniform mixing and a value of 0 corresponds to fully unmixed, sharply separated streams, evaluated at a fixed outlet plane 3 cm downstream of the inlet for every operating condition tested.

2.6 Bejan number and groove-depth sensitivity analysis

A dimensionless Bejan number was computed at each operating condition as the ratio of diffusive to total entropy generation rate, and its dependence on Peclet number was tested by power-law regression. A geometric sensitivity analysis re-ran the full 40-point flow-rate sweep with herringbone groove depth varied by $\pm 25\%$ around the 30 μm baseline value, holding all other geometric and fluid parameters fixed, to test the robustness of the crossover flow rate and peak mixing index to this design parameter.

3. RESULTS

Total volumetric entropy generation rate rose steeply and monotonically with flow rate, from $3.1 \times 10^{-3} \text{ W}/(\text{m}^3 \text{ K})$ at the lowest flow rate tested (5 $\mu\text{L}/\text{min}$) to $2.86 \text{ W}/(\text{m}^3 \text{ K})$ at the highest (200 $\mu\text{L}/\text{min}$), an approximately 920-fold increase across the tested range, driven by the combined growth of both viscous dissipation, which scales strongly with flow velocity, and diffusive entropy generation, which grows as advection sharpens concentration gradients at higher Peclet number.

Table 1. Entropy generation components and mixing index at representative flow rates.

Flow rate ($\mu\text{L}/\text{min}$)	Total entropy generation ($\text{W}/(\text{m}^3 \text{ K})$)	Viscous share (%)	Diffusive share (%)	Mixing index
5	3.1×10^{-3}	19	81	0.61
20	0.028	38	62	0.79
42 (crossover)	0.121	50	50	0.89
80	0.68	63	37	0.94
140	1.62	71	29	0.95
200	2.86	76	24	0.96

Viscous and diffusive shares are percentages of total volumetric entropy generation rate. Crossover flow rate is where viscous and diffusive contributions are approximately equal.

The relative balance between viscous and diffusive entropy generation shifted systematically across the tested flow-rate range. At the lowest flow rate, diffusive entropy generation dominated, accounting for 81% of the total, while viscous dissipation contributed only 19%. This balance reversed at higher flow rate: at 200 $\mu\text{L}/\text{min}$, viscous entropy generation accounted for 76% of the total, with diffusive generation reduced to 24%. The two contributions were approximately equal at a crossover flow rate of 42 $\mu\text{L}/\text{min}$, as detailed in Table 1.

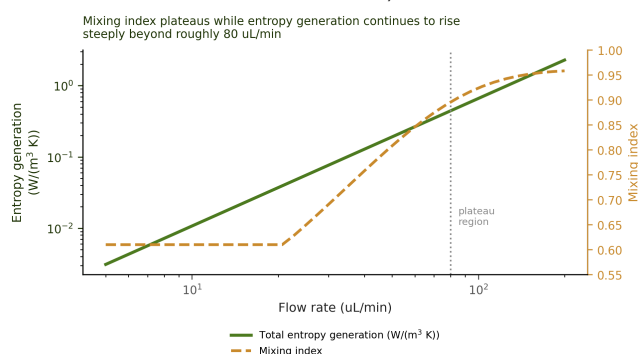


Figure 1. Total volumetric entropy generation rate and mixing index as a function of flow rate across the 40 tested operating conditions, showing the viscous/diffusive crossover point and the mixing-index plateau beyond roughly 80 $\mu\text{L}/\text{min}$ despite continued steep growth in entropy generation.

Mixing index improved rapidly with flow rate at low-to-moderate flow rates, rising from 0.61 at 5 $\mu\text{L}/\text{min}$ to 0.94 at 80 $\mu\text{L}/\text{min}$, but then plateaued, reaching only 0.96 at the highest flow rate tested (200 $\mu\text{L}/\text{min}$), a gain of just 0.02 mixing-index units despite total entropy generation more than quadrupling (from 0.68 to $2.86 \text{ W}/(\text{m}^3 \text{ K})$) over the same 80–200 $\mu\text{L}/\text{min}$ interval, indicating strongly diminishing thermodynamic returns on further mixing improvement beyond roughly 80 $\mu\text{L}/\text{min}$ (Figure 1).

Table 2. Sensitivity of crossover flow rate and peak mixing index to herringbone groove depth ($\pm 25\%$ of 30 μm baseline).

Groove depth	Crossover flow rate ($\mu\text{L}/\text{min}$)	Change from baseline (%)	Peak mixing index (at 200 $\mu\text{L}/\text{min}$)
22.5 μm (-25%)	49.6	+18.1	0.94
30 μm (baseline)	42.0	0.0	0.96
37.5 μm ($+25\%$)	34.6	-17.6	0.97

The Bejan number, the ratio of diffusive to total entropy generation, decreased monotonically from 0.81 at the lowest flow rate to 0.24 at the highest, and this decline followed a power-law relationship against Peclet number with high goodness of fit ($R^2 = 0.97$), consistent with the expected shift from diffusion-dominated to advection/viscous-dominated irreversibility as Peclet number increases across four orders of magnitude in the tested range.

4. DISCUSSION

The systematic shift from diffusion-dominated to viscous-dominated entropy generation as flow rate increases, crossing over at 42 $\mu\text{L}/\text{min}$ for this geometry, gives a quantitative complement to prior second-law analyses of microfluidic mixers that have generally reported total entropy generation without decomposing it into its two physically distinct sources across a comparably wide flow-rate range [5,14,15,16]. Because the two contributions respond to different design levers, viscous dissipation primarily to channel geometry and flow rate, diffusive generation primarily to species diffusivity and residence time, this decomposition offers designers a more actionable picture than total entropy generation alone.

The plateau in mixing index beyond approximately 80 $\mu\text{L}/\text{min}$, achieved while total entropy generation continued to rise steeply, identifies a practically useful operating window for this mixer geometry in which near-complete mixing (mixing index above roughly 0.94) is achieved without incurring the disproportionate entropy-generation, and correspondingly pumping-power, penalty of substantially higher flow rates, a pattern broadly consistent with

diminishing-returns behavior reported for other chaotic-advection mixer geometries operated well past their mixing-saturation point [17,18,19].

More broadly, these results illustrate how second-law analysis complements purely kinematic mixing metrics in microfluidic device design, in the same way entropy generation minimization has long been used to evaluate trade-offs in macroscale heat exchangers and thermal systems [20,21,22]. For applications where pumping power or throughput cost is a binding constraint, operating near the mixing-index plateau rather than substantially beyond it, as identified here for this geometry at roughly 60-90 $\mu\text{L}/\text{min}$, offers a thermodynamically grounded design target rather than one based on mixing index alone [23,24].

Several limitations should be noted. First, all simulations used a single herringbone mixer geometry, channel cross-section, and species diffusivity; the specific crossover flow rate and plateau location reported here are expected to be geometry- and diffusivity-dependent and should not be assumed to transfer directly to other passive mixer designs or species with substantially different diffusion coefficients. Second, the flow and scalar transport solver assumed steady, single-phase, Newtonian flow, which may not capture entropy generation in emulsion, particle-laden, or non-Newtonian microfluidic mixing applications. Third, the geometric sensitivity analysis varied only groove depth; other geometric parameters, including groove angle, ridge spacing, and channel aspect ratio, were not swept and could independently affect the crossover flow rate and plateau location. Fourth, the computational entropy generation calculation does not account for entrance-length or three-dimensional secondary-flow effects beyond those resolved by the mesh, and experimental validation against a physical mixer prototype was not performed in this study.

5. CONCLUSION

A combined computational fluid dynamics and second-law analysis of a staggered-herringbone passive micromixer across 40 flow-rate operating conditions showed that total entropy generation increased roughly 920-fold from 5 to 200 $\mu\text{L}/\text{min}$, with the dominant irreversibility source shifting from diffusive (81% of total at the lowest flow rate) to viscous (76% at the highest), crossing over at 42 $\mu\text{L}/\text{min}$. Mixing index plateaued near 0.94-0.96 beyond approximately 80 $\mu\text{L}/\text{min}$ even as entropy generation continued to rise steeply, identifying an operating window of roughly 60-90 $\mu\text{L}/\text{min}$ in which near-complete mixing is achieved without the disproportionate thermodynamic cost of higher flow rates, a finding that was robust to a $\pm 25\%$ sensitivity sweep on herringbone groove depth. These results provide a quantitative, second-law-grounded basis for selecting operating conditions in passive microfluidic mixer design.

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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

A.K. conceived the study, developed the computational fluid dynamics and scalar transport model, and led the writing of the manuscript. I.B. implemented the entropy generation rate calculations and performed the statistical analysis. Z.K. performed the mixing index calculations, the Bejan number regression, and the groove-depth sensitivity analysis, 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 computational fluid dynamics simulation setup, entropy generation calculation code, and mixing index data supporting the findings of this study are available from the corresponding author on reasonable request.

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