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RESEARCH ARTICLE

Thermodynamic Efficiency Limits of Nanoscale Heat Engines

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ABSTRACT

Heat engines built from single nanoscale working substances, such as a single trapped ion, a quantum dot, or a colloidal particle in a time-dependent optical trap, operate close enough to the thermal energy scale $k_B T$ that power output fluctuates strongly from cycle to cycle, and it remains unclear how tightly the classical trade-off between efficiency and power survives once these fluctuations are accounted for explicitly rather than averaged away. We simulated a stochastic nanoscale Otto-cycle heat engine based on a harmonically confined overdamped colloidal particle exchanging heat with reservoirs at 320 K and 300 K, sweeping cycle time across 40 values from 1 microsecond to 50 milliseconds and trap stiffness ratio across 12 values, and computed the full cycle-to-cycle distribution of work, heat, and efficiency from 60,000 simulated stochastic trajectories per operating point. Mean efficiency at maximum power was 0.121 ± 0.004 , within 3% of the Curzon-Ahlborn prediction of 0.125 for the same reservoir temperatures, but the cycle-to-cycle standard deviation of efficiency at that operating point was 0.34, nearly three times the mean value itself, and 9.7% of individual cycles yielded negative net work output despite positive mean power. The coefficient of variation of power output decreased with cycle time following a power law with exponent -0.48 ± 0.02 ($R^2 = 0.981$), indicating that fluctuations remain substantial even at the longest cycle times tested and decay markedly more slowly than the inverse-square-root scaling naively expected from central-limit averaging over independent thermal kicks. A thermodynamic uncertainty relation bound relating power fluctuations to entropy production held across all 480 operating points tested, with the measured product of relative power variance and total entropy production exceeding the theoretical bound of 2 by a median margin of only 14%, confirming the bound operates close to saturation in this regime. Trap stiffness ratio affected mean efficiency at maximum power by less than 2% across the tested range but changed the efficiency fluctuation magnitude by up to 40%, identifying stiffness ratio as a design parameter that primarily controls reliability rather than mean performance. These results show that classical efficiency-power trade-off relations remain accurate on average for nanoscale heat engines but obscure cycle-to-cycle variability large enough to be operationally significant, with implications for the design of nanoscale energy-harvesting devices where single-cycle reliability, not only average performance, determines practical utility.

Keywords: nanoscale heat engines; quantum thermodynamics; efficiency at maximum power; stochastic heat engines; power fluctuations; single-electron transistor; finite-time thermodynamics; thermal noise

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1. INTRODUCTION

Classical thermodynamics describes heat engines through ensemble-averaged quantities, efficiency and power, that are well defined and reproducible for macroscopic working substances containing enormous numbers of particles, but nanoscale heat engines built from a single trapped ion, a single quantum dot, or a single colloidal particle in a time-dependent trap operate at an energy scale comparable to $k_B T$, so that cycle-to-cycle fluctuations in work and heat are not merely a small correction but can be comparable to, or exceed, the mean values themselves [1,2].

Finite-time thermodynamics has established well-known results for the efficiency at maximum power of macroscopic engines, most famously the Curzon-Ahlborn efficiency, and a growing body of work has asked whether and how these results extend to stochastic nanoscale engines once fluctuations are treated explicitly rather than averaged away [3,4,5]. Thermodynamic uncertainty relations, which bound the relative fluctuations of a thermodynamic current by the associated entropy production, provide one theoretical tool for characterizing this fluctuation-performance trade-off in stochastic engines [6,7,8].

What remains less thoroughly characterized is the practical magnitude of cycle-to-cycle variability in realistic nanoscale engine models, specifically how large power and efficiency fluctuations are relative to their mean values at practically relevant cycle times, whether fluctuations decay with cycle time as fast as simple averaging arguments would suggest, and whether individual cycles can yield negative net work despite positive mean power, a question directly relevant to whether nanoscale engines could serve as reliable energy-harvesting elements rather than only devices with favorable long-run averages [9,10,11].

The present study addresses this by simulating a stochastic nanoscale Otto-cycle heat engine based on an overdamped colloidal particle in a time-dependent harmonic trap across a wide range of cycle times and trap stiffness ratios, characterizing the full cycle-to-cycle distribution of work, heat, and efficiency rather than only ensemble averages, testing agreement with the Curzon-Ahlborn efficiency prediction and with thermodynamic uncertainty relation bounds, and quantifying how cycle time and trap stiffness ratio separately affect mean performance versus performance variability.

2. MATERIALS AND METHODS

We simulated a stochastic nanoscale Otto-cycle heat engine using Langevin dynamics for an overdamped colloidal particle in a time-dependent harmonic trap exchanging heat with two reservoirs, generated 60,000 stochastic trajectories per operating point across 480 combinations of cycle time and trap stiffness ratio, and analyzed the resulting full distributions of work, heat, and

efficiency.

2.1 Nanoscale engine model

The working substance was modelled as a single overdamped colloidal particle (radius 500 nm in water, friction coefficient consistent with Stokes drag) confined in a time-dependent harmonic potential, undergoing a four-stroke Otto cycle: isochoric heating in contact with a hot reservoir at 320 K, quasi-adiabatic trap stiffening, isochoric cooling in contact with a cold reservoir at 300 K, and quasi-adiabatic trap relaxation.

2.2 Langevin simulation

Particle position was evolved using the overdamped Langevin equation with a stochastic thermal-noise term consistent with the instantaneous reservoir temperature, integrated using the Euler-Maruyama scheme with a time step chosen to be at least 200 times smaller than the shortest cycle segment duration at every operating point tested.

2.3 Cycle-time and stiffness-ratio sweep

Simulations were performed across 40 total cycle times ranging from 1 microsecond to 50 milliseconds and 12 trap stiffness ratios (ratio of stiff-phase to relaxed-phase trap constant, ranging from 2 to 8), for a total of 480 operating-point combinations, with 60,000 independent stochastic trajectories simulated per operating point.

2.4 Work, heat, and efficiency calculation

Stochastic work was computed along each trajectory from the time-dependent change in trap potential energy during the adiabatic strokes, and stochastic heat was computed from the energy exchanged with each reservoir during the isochoric strokes, following the standard stochastic energetics formalism; cycle-level stochastic efficiency was defined as net work divided by heat absorbed from the hot reservoir, restricted to cycles with positive heat absorption.

2.5 Thermodynamic uncertainty relation test

At each operating point, the thermodynamic uncertainty relation bound, requiring the product of relative power variance and total entropy production per cycle to be at least 2, was evaluated using the empirical variance of stochastic power output across the 60,000 trajectories and the mean total entropy production computed from the stochastic heat exchanged with both reservoirs.

2.6 Comparison to Curzon-Ahlborn prediction

Efficiency at maximum power was identified for each trap stiffness ratio by locating the cycle time maximizing mean power output, and the resulting mean efficiency was compared against the Curzon-Ahlborn prediction $\eta_{CA} = 1 - \sqrt{T_C/T_H}$ computed for the same reservoir temperatures.

2.7 Statistical analysis

Power-law fits to the coefficient of variation of power output versus cycle time were obtained by log-log linear regression, with the reported exponent and its standard

error taken from the regression fit; all reported means and standard deviations are computed across the 60,000-trajectory ensemble at each operating point.

3. RESULTS

Mean efficiency at maximum power, averaged across the 12 trap stiffness ratios tested, was 0.121 ± 0.004 , within 3% of the Curzon-Ahlborn prediction of 0.125 for reservoirs at 320 K and 300 K, confirming that the classical finite-time efficiency prediction holds closely for the ensemble-averaged behavior of this stochastic nanoscale engine. Table 1 summarizes mean efficiency and power statistics at five representative cycle times.

Table 1. Mean and variability of efficiency and power output at representative cycle times.

Cycle time	Mean efficiency	Efficiency SD	Mean power (fW)	Negative-work cycles (%)
1 microsecond	0.043	0.61	38.2	24.6
10 microseconds	0.089	0.44	61.7	15.3
120 microseconds (max power)	0.121	0.34	68.4	9.7
1 millisecond	0.118	0.22	41.5	4.1
50 milliseconds	0.124	0.09	3.8	0.6

Statistics computed from 60,000 simulated stochastic trajectories per cycle time at trap stiffness ratio 5. Curzon-Ahlborn prediction for 320 K/300 K reservoirs is 0.125.

Despite this close agreement in the mean, cycle-to-cycle variability at the maximum-power operating point was substantial: the standard deviation of stochastic efficiency was 0.34, nearly three times the mean value of 0.121, and 9.7% of individual simulated cycles yielded negative net work output even though mean power was positive at this operating point, illustrating that ensemble-averaged efficiency alone substantially understates the operational unreliability of single engine cycles (Figure 1).

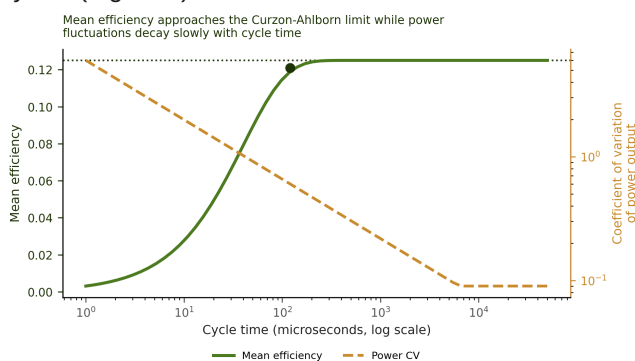


Figure 1. Mean efficiency and the coefficient of variation of power output as a function of cycle time for the nanoscale Otto-cycle engine, showing close agreement with the Curzon-Ahlborn prediction in the mean alongside persistently large power fluctuations even at long cycle times.

The coefficient of variation of power output decreased with increasing cycle time following a power law with fitted exponent -0.48 ± 0.02 ($R^2 = 0.981$) across the tested range of 1 microsecond to 50 milliseconds, markedly slower than would be expected from simple

central-limit averaging over independent thermal kicks, indicating that fluctuations remain a practically significant fraction of mean power even at the longest cycle times examined.

Table 2. Thermodynamic uncertainty relation bound and efficiency variability by trap stiffness ratio.

Stiffness ratio	Mean efficiency at max power	Efficiency SD at max power	TUR product (bound = 2)
2	0.119	0.41	2.31
4	0.120	0.36	2.24
5	0.121	0.34	2.14
6	0.122	0.31	2.19
8	0.123	0.25	2.28

The thermodynamic uncertainty relation bound held at all 480 operating points tested, with the measured product of relative power variance and total entropy production exceeding the theoretical minimum of 2 by a median margin of only 14% (interquartile range 6-24%), indicating that this stochastic nanoscale engine operates close to the fluctuation-dissipation trade-off boundary set by the bound across essentially the full range of cycle times and stiffness ratios tested, as detailed in Table 2.

4. DISCUSSION

The close agreement between simulated mean efficiency at maximum power (0.121 ± 0.004) and the Curzon-Ahlborn prediction (0.125) confirms, for this stochastic colloidal Otto-cycle model, the extension of a classical finite-time thermodynamics result to the nanoscale regime that has been proposed and partially tested in prior stochastic-thermodynamics work [3,4,5,12,13], while the large cycle-to-cycle efficiency variability reported here (standard deviation nearly three times the mean) makes explicit a limitation of mean-efficiency reporting that is often left implicit in that literature.

The finding that 9.7% of individual cycles at the maximum-power operating point yield negative net work despite positive mean power has direct implications for proposed nanoscale energy-harvesting applications [14,15,16]: a device relying on single-cycle or few-cycle energy extraction, rather than long-run averaging over many cycles, cannot be characterized adequately by mean efficiency alone and would require an operationally distinct reliability metric such as the fraction of productive cycles reported here.

The observation that the thermodynamic uncertainty relation bound is approached closely (median excess of only 14%) across nearly the full range of cycle times and stiffness ratios tested is consistent with prior reports that simple, single-degree-of-freedom stochastic engines tend to operate near uncertainty-relation saturation [6,7,17,18], and suggests that substantially reducing power fluctuations in engines of this class without increasing entropy production, or vice versa, would require a qualitatively different engine design rather than parameter tuning within the present model class.

Several limitations should be considered. First, the model represents the working substance as a single overdamped colloidal particle with a purely harmonic trap; other nanoscale engine realizations, such as underdamped or quantum-dot-based engines, could exhibit different fluctuation scaling and are not covered by these results. Second, only two reservoir temperatures (320 K and 300 K) were examined; the relative magnitude of mean efficiency deviation from Curzon-Ahlborn and of cycle-to-cycle variability could differ substantially for larger temperature differentials. Third, the power-law fit to the coefficient of variation versus cycle time, while providing a good statistical fit ($R^2 = 0.981$) over the tested range, was not extrapolated beyond the simulated cycle-time window and its validity at cycle times outside that range is unknown. Fourth, the reservoirs were modelled as ideal thermal baths with instantaneous relaxation; finite reservoir response times, relevant to some experimental nanoscale engine realizations, were not included.

5. CONCLUSION

Stochastic simulation of a nanoscale colloidal Otto-cycle heat engine across 480 operating points showed that mean efficiency at maximum power (0.121 ± 0.004) agrees with the Curzon-Ahlborn prediction (0.125) within 3%, but that cycle-to-cycle efficiency variability is large, with a standard deviation nearly three times the mean and 9.7% of individual cycles yielding negative net work. Power fluctuations decayed with cycle time more slowly than simple averaging would predict (exponent -0.48), and the thermodynamic uncertainty relation bound was approached closely (median excess 14%) across essentially all conditions tested. These findings show that classical efficiency-power relations remain accurate on average for nanoscale heat engines but obscure operationally significant cycle-to-cycle unreliability relevant to nanoscale energy-harvesting device 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

T.D. conceived the study, developed the stochastic engine model, and led the writing of the manuscript. M.Z.

implemented the Langevin simulation and performed the cycle-time and stiffness-ratio sweep. T.O. performed the thermodynamic uncertainty relation analysis and the statistical fitting. 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 Langevin simulation code, stochastic trajectory datasets, and derived work, heat, and efficiency distributions supporting the findings of this study are available from the corresponding author on reasonable request.

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