

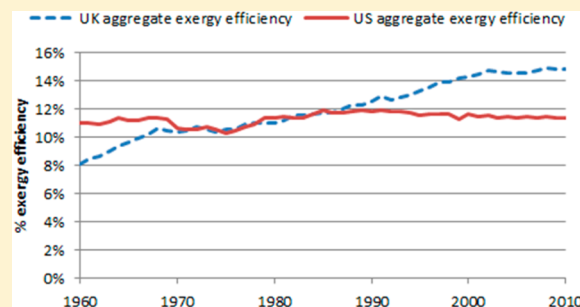
Divergence of Trends in US and UK Aggregate Exergy Efficiencies 1960–2010

Paul E. Brockway,* John R. Barrett, Timothy J. Foxon, and Julia K. Steinberger

Sustainability Research Institute, School of Earth and Environment, University of Leeds, Leeds LS2 9JT, United Kingdom

S Supporting Information

ABSTRACT: National exergy efficiency analysis relates the quality of primary energy inputs to an economy with end useful work in sectoral energy uses such as transport, heat and electrical devices. This approach has been used by a range of authors to explore insights to macroscale energy systems and linkages with economic growth. However, these analyses use a variety of calculation methods with sometimes coarse assumptions, inhibiting comparisons. Therefore, building on previous studies, this paper first contributes toward a common useful work accounting framework, by developing more refined methodological techniques for electricity end use and transport exergy efficiencies. Second, to test this more consistent and granular approach, these advances are applied to the US and UK for 1960 to 2010. The results reveal divergent aggregate exergy efficiencies: US efficiency remains stable at around 11%, while UK efficiency rises from 9% to 15%. The US efficiency stagnation is due to “efficiency dilution”, where structural shifts to lower efficiency consumption (e.g., air-conditioning) outweigh device-level efficiency gains. The results demonstrate this is an important area of research, with consequent implications for national energy efficiency policies.



1. INTRODUCTION

Energy efficiency has been an important global issue since the 1970s, when energy security issues stemming from the 1973 oil crisis triggered the formation of the International Energy Agency (IEA) in 1974, prompting seminal research into national energy efficiency (e.g., refs 1 and 2). We distinguish between energy efficiency, which relates energy inputs and outputs, and energy intensity, which relates energy use to economic outputs (e.g., primary energy/GDP, see ref 3).

National energy efficiency analysis plays a key role in advancing research into energy issues, including energy projections. It does this by studying first technology use at device levels and second energy consumption at economic sector (e.g., residential/commercial, industry and transport) and aggregate levels. Exergy and useful work analysis is distinct from traditional “first law” energy analysis by accounting for the quality of energy, thus incorporating the degradation of useful energy according to the second law of thermodynamics. This also enables the linking of macro- and microscale efficiency analysis to give a complete energy picture of an economy, enabling additional insight into energy use and drivers of change. These aspects are important for understanding the role of exergy inputs and conversion efficiency improvements as drivers of economic growth.^{4,5}

Exergy, a term introduced in 1956 by Rant,⁶ is simply defined as “available energy”.² “Availability” is a key thermodynamic concept: the second law of thermodynamics means not all input energy is transformed into work, and thus exergy is lost during energy conversion processes. A heat engine provides a

classic second law example, as the maximum thermodynamic efficiency is the Carnot temperature ratio $(1 - T_2/T_1)$. The main classes of “work” in national exergy analyses are heat, mechanical drive (e.g., transport), muscle work and electricity uses. We use the “task-level” terminology introduced by Carnahan et al.¹ to refer to work in subclass applications (e.g., room heating), rather than use “subsector” to avoid confusion with economic terminology. It also allows us to adopt their “useful work” definition as “the minimum exergy input to achieve that task work transfer”.¹ Task-level exergy efficiency is therefore:

$$\begin{aligned} \epsilon_{\text{task}} &= \frac{\text{useful work}}{\text{primary exergy}} \\ &= \frac{\text{min exergy input to achieve task work transfer } (B_{\text{min}})}{\text{max reversible work done as system reaches equilibrium } (W_{\text{max}})} \end{aligned} \quad (1)$$

Figure 1 helps visualize the difference between first law energy efficiency, η , and second law exergy efficiency, ϵ . In the example, a gas boiler heats an internal room to 20 °C, with an outdoor temperature of 5 °C. Due to the Carnot temperature ratio penalty, the second law efficiency, $\epsilon = \eta(1 - T_{\text{outside}}/T_{\text{room}}) = 4.1\%$, significantly lower than the 80% first law boiler efficiency.

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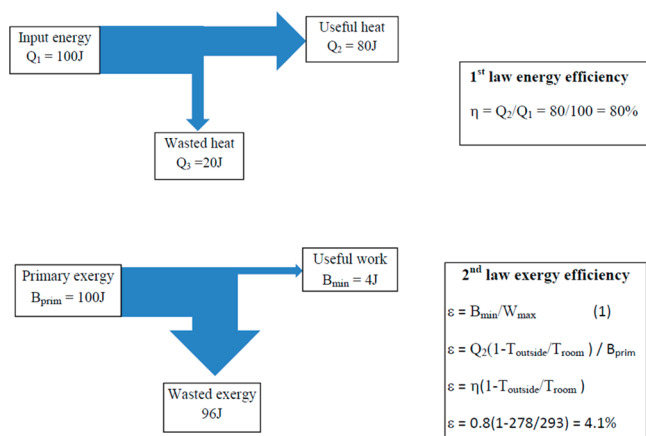


Figure 1. Energy (1st law) versus exergy (2nd law) efficiency for typical domestic boiler heating system.

Exergy therefore flows through a national economy, starting with primary exergy, reducing to a smaller exergy value at its transformed end use stage (e.g., heat), which is considered as “useful work” to the economy. At this point, it is consumed to help produce a final “energy service” (e.g., passenger-km or thermal comfort). In the last stage, any remaining exergy dissipates to zero by reaching thermodynamic balance with its surroundings. As useful work is the last stage measurable in energy units (joules) within a consistent exergy analysis framework, we focus on primary exergy and useful work, and not energy services. The resulting exergy efficiencies (ratios between 0 and 1) measure energy quality in terms of the efficiency with which the exergy content of primary energy sources is converted to useful work. This paper measures aggregate exergy efficiency at a national level, which is simply the sum of all task-level useful work divided by total input exergy:

$$\varepsilon_{\text{tot}} = \frac{\sum \text{useful work}}{\sum \text{primary exergy}} \quad (2)$$

Significant effort has been expended on national exergy analysis since Reistad’s 1970 US analysis,² with single year analyses published at country (e.g., refs 7–10) and global levels.^{11,12} Time-series national exergy analyses are rarer due to data availability, but have most notably been undertaken by Ayres, Warr and colleagues who estimated 1900–2000 aggregate efficiencies for the US, UK, Japan and Austria.^{13–15} Most recently, Serrenho et al.^{16,17} published analysis covering Portugal 1859–2009 and EU-15 countries 1960–2009.

Despite exergy analysis’s advantage that it “quantifies the locations, types and magnitudes of [energy] wastes and losses”,¹⁸ it remains the poor relation of energy analysis, with a key issue being the need for methodological consistency to improve comparability of results. This paper seeks to address this issue. First, it builds on recent efforts by Serrenho et al.¹⁶ toward a common accounting framework using IEA input energy data, which represents the state-of-the-art in comparable worldwide energy data, by developing more granular techniques for electricity end use and transport (mechanical drive) efficiencies. Second, the improved methodology is then applied to UK and US exergy and useful work analyses for the period 1960–2010, aligning with input IEA energy data availability. The US and UK are chosen as they were previously analyzed for the period 1900–2000 by Warr et al.,^{15,19} allowing

comparisons and insights into postindustrial energy use patterns.

We align our analysis with the energy carriers boundary taken by Ayres et al.¹³ and Serrenho et al.,¹⁶ meaning the main appropriated energy flows intended for energy use are considered: coal, gas, oil, nuclear, food (for manual labor), combustible renewables, hydropower and other renewables. The alternative biophysical approach, adopted by Scuibba²⁰ and Krausmann et al.,²¹ includes material flows (e.g., cotton, iron ores) that are both outside our energy carriers boundary and have a minimal contribution ($\sim 2\%$ for the Chen et al. China²² analysis). Our useful work analysis is distinct from the important field of energy services (e.g., refs 23 and 24), and while we use “device” (i.e., domestic boiler) energy transfer efficiencies, we do not explicitly include passive systems (e.g., house or insulation) in our analysis.

The paper is structured as follows: section 2 describes Methods, Results are in section 3 and a Discussion is given in section 4. The Supporting Information contains more detail on the mapping categories to useful work, exergy to useful work calculations and postresults analysis.

2. METHODS

The basic useful work accounting method follows Ayres and Warr’s (e.g., ref 15) approach. Their method, well documented in sections 3 and 4 of their book “The Economic Growth Engine”,²⁵ is based on five key steps. First, national-level primary energy data (i.e., oil, coal, gas, nuclear, renewables, food and feed) is converted back to primary exergy via “chemical equivalent” conversion factors for fossil fuels²⁶ and technology conversion values for renewables. In step 2, the primary exergy values (by energy type) are mapped to task levels within each main useful work category (heat, mechanical drive, electricity and muscle work). For example, work done by cars, trucks, aircraft and rail are task levels within the mechanical drive category. Step 3 establishes task-level conversion efficiencies, using published values or new estimations. In step 4, individual task-level useful work by energy source is calculated by multiplying task-level inputs and conversion efficiencies from steps 2 and 3. Finally, step 5 calculates the overall national exergy efficiency value by summing end useful work and dividing by total primary exergy inputs (eq 2).

Serrenho et al.¹⁶ made significant advances to the approach in steps 1 and 2 by standardizing the primary energy mapping to useful work categories based on IEA data sets.²⁷ This paper follows the IEA mapping approach for the US and UK analyses, as shown in the Supporting Information. The IEA energy data may differ from national data sets, but such differences are typically small ($<5\%$), and being based on a single methodology greatly strengthens cross-country comparisons. This paper proposes methodological advances for task-level exergy efficiencies within step 3, to help build a common analytical useful work accounting framework. The main features are given below, with more detailed descriptions in the Supporting Information.

The first major revision is to electricity, giving more granular treatment to electricity end uses. Originally, Ayres and Warr categorized electricity as pure work,¹³ so electricity exergy efficiency was just equal to electricity generation efficiency ($\sim 35\%$). Subsequently, Ayres et al.²⁸ estimated task-level efficiencies for end uses of electricity, by including end-use device efficiencies for motors, heating, cooling and cooking, and

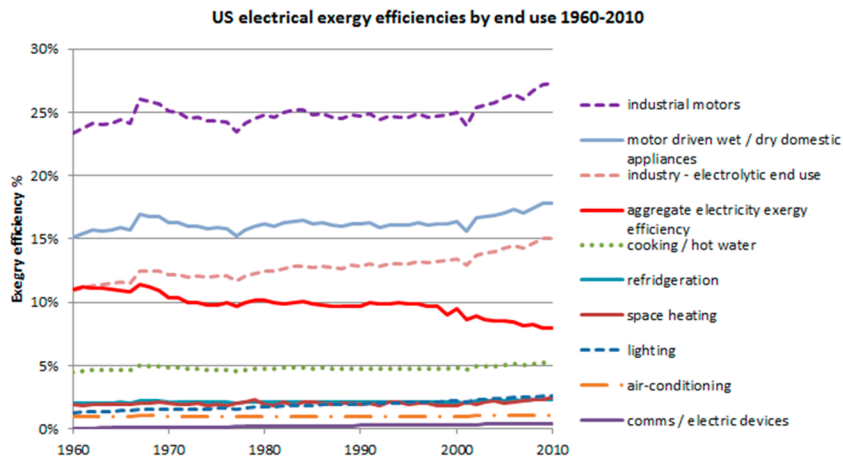


Figure 2. US electricity exergy efficiencies by end use 1960–2010.

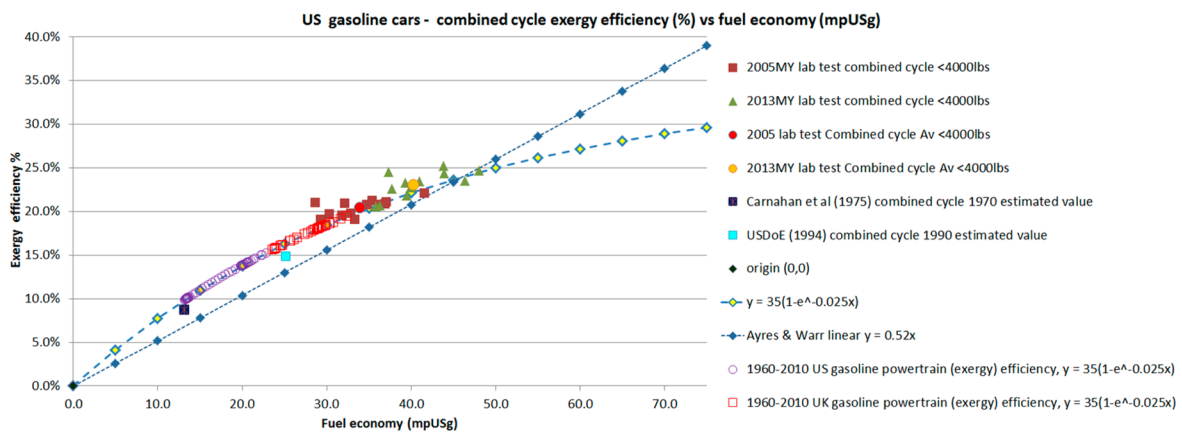


Figure 3. US gasoline cars (mechanical drive) empirically derived exergy efficiency (%) vs fuel economy (mpg).

these were incorporated into national exergy analyses.^{15,16} We make two important changes, which reduce the overall electricity exergy efficiency. First, we include Carnot temperature ratio penalties for electrical high temperature heat (HTH), refrigeration and air-conditioning, omitted from previous studies (e.g., Figure 4.19, ref 25), to match the second law approach of other heating/cooling applications. Second, we provide more granular mapping of IEA electricity consumption to main end uses (e.g., electric motors, heat, electrical appliances, computers, lighting) within each main economic sector (e.g., industry, commerce, residential) based on local country end use consumption data.^{29,30} Particular attention is given to adding granularity to residential electricity use, a significant and growing proportion of total electricity consumption (see the Supporting Information), including household appliance exergy efficiency calculations. Electricity exergy efficiencies are then equal to electrical generation efficiency multiplied by electrical end-use device efficiencies. These methodological changes reveal a dilution effect within electricity usage, shown in Figure 2 for the US: overall electricity exergy efficiency decreases from 11% to 8% over time, as structural shifts to less efficient electricity uses (e.g., air conditioning) occur faster than task-level efficiencies rise for each electricity end use type.

Second, a novel approach is developed for mechanical drive (transport) to improve the estimation of time-series exergy efficiency in this important sector, which forms ~30% of total primary energy demand. Traditional techniques (e.g., refs 9 and

15) follow Carnahan et al.,³¹ where overall exergy efficiency is derived from thermal engine efficiency (~30%) multiplied by assumed (~30%) postengine losses (e.g., heat, internal friction and other drive-line losses), leaving the estimated exergy efficiency at 8%–10% for a typical car. Although some engine efficiencies have been tracked over time, postengine loss factors have not, resulting in arbitrary judgment about their time-series variation.

Ayres et al.¹³ adopted a road transport exergy efficiency, $\epsilon = 0.52 \times \text{mpg}$ as a proxy for mechanical drive efficiency, as improved fuel economy (in miles per gallon (mpg)) is assumed to reflect increases in power-train efficiency. We advance this approach, by estimating exponential curves that relate exergy efficiency as a function of vehicle fuel economy, for all UK and US major transport modes (road, rail, air) during the period 1960–2010. Our method is based on a detailed investigation of US gasoline cars, because this transport mode had the most detailed source data, from Oak Ridge National Laboratory, who had measured power-train force and fuel economy for 68 US road vehicles.³² Power-train force is the residual force available at the wheels after engine, idling, drive-train and parasitic losses are incurred (note all power-train force is dissipated subsequently via drag, tire rolling and braking losses). It is estimated by the US Department of Energy (USDoe) to be 14–26% of starting fuel energy (primary exergy) for new cars, depending on drive cycle.³³ Dynamometer power-train results enabled useful work (power-train tractive force \times distance traveled), and thus exergy efficiency (useful work/primary

exergy), to be calculated for all vehicle test data for Model Year (MY) 2005 and MY 2013. To estimate a best-fit curve for the whole period, we combine these results with the estimates of vehicle exergy efficiencies from 1970 (Reistad)³¹ and 1994 (USDoe),³⁴ and an estimated maximum exergy efficiency of 35% for gasoline cars (assuming current best practice engine thermal efficiency = future limiting exergy efficiency). This gives an empirical best-fit inverse exponential $\varepsilon = 35(1 - e^{-0.025x})$ relating exergy efficiency ε to fuel economy x (in mpg), shown in Figure 3. We acknowledge the lack of historical data prior to 2005 (except single point 1970 and 1994 values) is a weakness, and would redraw the best-fit curve if such historical data was found. Nevertheless, it represents progress against the incumbent arbitrary loss factor or linear ε -mpg assumptions, and provides a better trajectory for future energy scenarios, where higher fuel economy values lie.

This approach was then extended to diesel-road, rail and air sectors using the same principle, i.e., fitting curves relating vehicle exergy efficiencies to fuel economy by combining historical and estimated maximum values. The fitted curves (plotted in the Supporting Information) enable exergy efficiencies (and hence useful work) to be estimated based on 1960–2010 UK and US fuel economy data.^{29,35–38}

The other analysis elements are largely similar to Ayres and Warr²⁵ and Serrenho et al.¹⁶ approaches. Heat is mapped to four task-levels: HTH at 600 °C; medium temperature heat (MTH2) at 200 and 100 °C (MTH1), and low temperature heat (LTH) at ~20 °C. For HTH, a weighted average of the two largest HTH consuming industrial sector efficiencies (steel and petrochemicals) is taken. MTH2 is lower temperature (~200 °C) industrial heat, which was estimated as the Carnot temperature pro-rata of the HTH efficiency (as no more specific data was available). For LTH and MTH1, the exergy efficiency is the assumed device (gas boiler) conversion ratio (70–90%) multiplied by the Carnot temperature ratio. Manual labor follows Serrenho et al.¹⁶ by calculating the amount of manual labor involved in human “mechanical drive” outputs (UK and US draft animals useful work contribution is negligible post-1960), and taking the additional manual labor calories into the exergy and useful work calculations. We also remove nonenergy uses of primary exergy from our analysis (e.g., bitumen and petrochemical feedstocks) as others (e.g., refs 10 and 25) have done. However, Serrenho et al.¹⁶ asks whether it should be included, and as nonenergy use is a small but growing sector, accounting for ~5% of primary energy demand, we discuss it further in the Supporting Information.

Incorporating these methodological changes, the national-level aggregate exergy efficiencies for the US and the UK are calculated on an annual basis for the period 1960–2010 using eq 2, following the five step approach summarized above (detailed in the Supporting Information). The exergy efficiency is calculated on the primary-to-useful basis adopted by Warr et al.,¹⁵ Nakicenovic et al.¹¹ and Reistad,² as opposed to the final-to-useful basis of Serrenho et al.¹⁶ The latter approach gives higher quoted efficiency values, because typical primary to final energy conversion efficiencies are 65–70%.

3. UK AND US EXERGY EFFICIENCY 1960–2010: RESULTS

Figure 4 shows the aggregate US exergy efficiency has remained stable at around 11% over the period 1960–2010. This stability is due to heat exergy efficiency gains (9% to 13%) being offset by reductions in electricity exergy efficiency (11% to 8%).

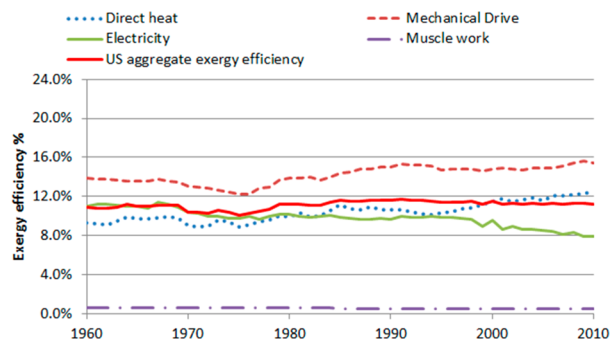


Figure 4. US exergy efficiency 1960–2010 by end use.

Muscle work has limited impact on the overall US efficiency due to the small size of its exergy and useful work contribution compared to that from heat, mechanical drive and electricity sectors (see the Supporting Information).

Figure 5 shows the UK aggregate exergy efficiency rose from 9% to 15%, with gains in all three main sectors: heat rose from

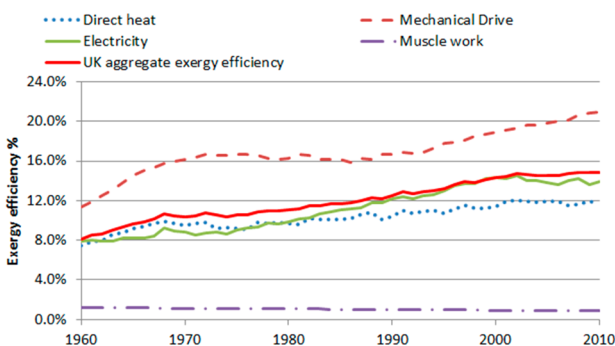


Figure 5. UK exergy efficiency 1960–2010 by end use.

8% to 12% (due to significant gains in all task-level efficiencies); electricity 8% to 14% (largely due to a rise in electricity generation efficiency from 30% to 43%) and mechanical drive 11% to 21% (due to dieselisation and increases in fuel economy). Task-level efficiency plots and electricity generation efficiencies are shown in the Supporting Information.

Figures 6 and 7 show the normalized plots of exergy, exergy efficiency and useful work versus a 1960 datum. The US exergy efficiency stagnation means the doubling of useful work in this period is almost all due to an increase in primary exergy. In contrast, the UK’s almost identical doubling of useful work

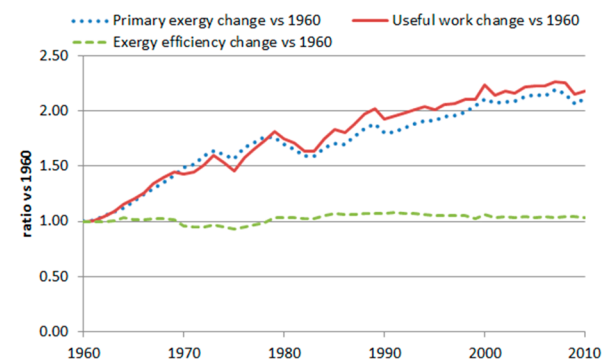


Figure 6. US normalized exergy, efficiency, useful work vs 1960.

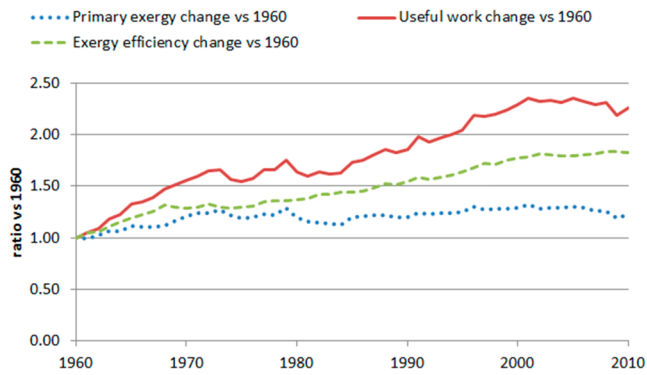


Figure 7. UK normalized exergy, efficiency, useful work vs 1960.

since 1960 has been mainly delivered by a large rise in exergy efficiency.

Figure 8 shows the 2010 flow diagram from primary exergy to useful work for the UK. It shows how 86% of the input primary exergy is lost and only 14% remains at the useful work stage. Useful work by end use is split fairly evenly between direct heat (30%), direct mechanical work (32%) and electricity end uses (38%). Manual mechanical work forms only 0.03% of total end useful work, reflecting the UK’s mature industrialized economy.

4. UK AND US EXERGY EFFICIENCY 1960–2010: DISCUSSION

The 50 year stagnation in overall US exergy efficiency is a striking and hitherto unexpected result. It has remained remarkably stable at around 11% since 1960, in contrast to the UK, which increased from 8.8% in 1960 to a 2008 peak of 15.0%. The divergence in UK–US overall exergy efficiencies occurred as the UK became more efficient in all three main

useful work categories: heat, electricity and mechanical drive, whereas US heat efficiency gains were offset by a large reduction in electricity efficiency.

The UK–US exergy efficiency divergence is revealed due to our methodological changes to electricity and mechanical drive. First, the more granular treatment of electricity task-level uses has more influence on US electrical exergy efficiency (largely owing to greater use of air-conditioning) and results in US electricity aggregate efficiency decreasing from 11.0% in 1960 to 7.9% in 2010. Second, by adopting our empirical ϵ -mpg approach for major transport modes, we assembled a time-history profile of task-level exergy efficiencies that represents a more robust improvement on previous strategies of either arbitrary loss-factor adjustments or linear ϵ -mpg relationships. The result is a more realistic time-series representation of task-level exergy efficiencies for transport: for example, as road-based fuel economy has remained static in the US since 1980,³⁴ due to the trend for larger and faster accelerating cars (and trucks), the derived US transport mechanical drive efficiencies have not increased, in contrast to the UK, where fuel economy and hence exergy efficiency (via the empirical relationship) has improved significantly.

The stagnating US national exergy efficiency appears to mimic the “efficiency dilution” effect first described in exergy analysis literature by Williams et al.¹⁴ for Japan. This is where greater use of lower efficiency processes (e.g., US air-conditioning has risen from 10% to 20% of electricity end use) outweigh task-level efficiency gains. It is most evident in the electricity sector, but similar shifts to lower efficiency processes also occurred in the US heat sector: HTH halved from 1960 to 2010 (due to declining manufacturing HTH use), while LTH increased 20% in the same period (due to gains in residential consumption). In the UK, dilution within heat and electricity sectors was more than offset by gains in task-level

UK 2010 Primary exergy to useful work flow map

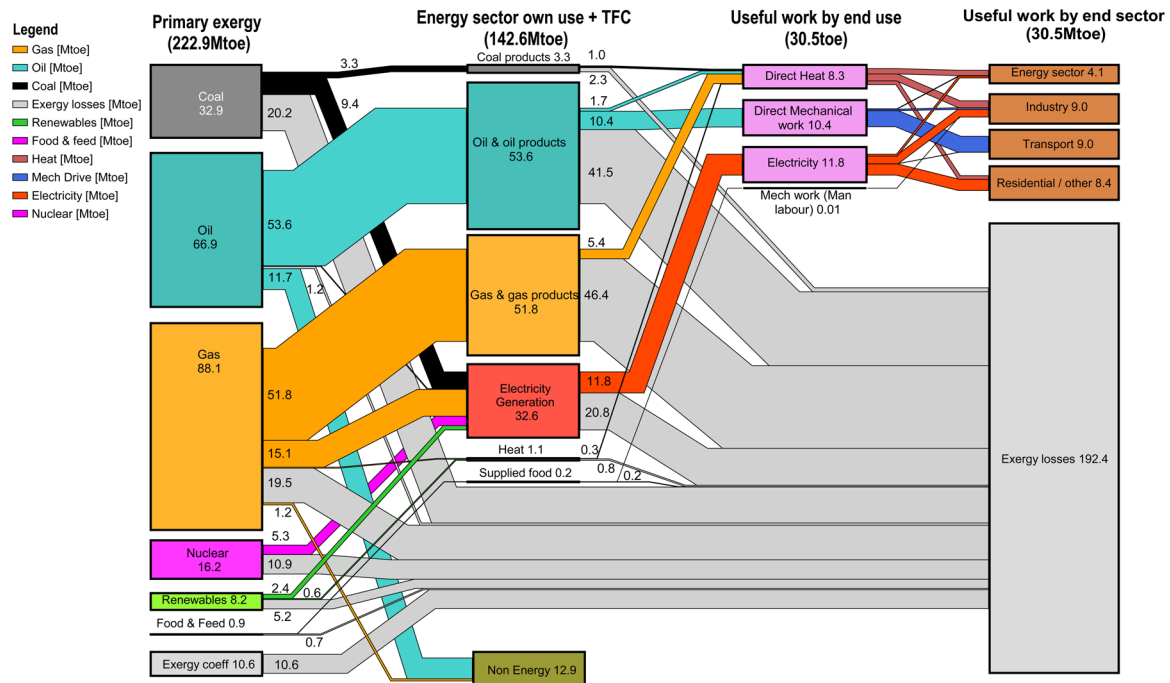


Figure 8. UK exergy to useful work flowchart (2010).

exergy efficiencies over this period. Nevertheless, UK heat and electricity efficiencies also peaked around 2000 (as with the US), and were stable to 2010. Compounding the structural dilution effect (e.g., shifting from HTH to LTH within heat sector) are approaching asymptotic device efficiency limits. Annual increases in task-level efficiencies are lower now than in 1960; for example, boiler (first law) efficiencies have increased from 70% toward an asymptotic limit somewhere over 90%. This highlights the importance of passive system analysis (e.g., ref 12), as this provides a larger energy reduction scope when reaching device efficiency limits.

Comparing our US results to earlier studies, Ayres and Warr^{15,25} estimated US efficiency in 1960 as 8%, lower than our result of 11%. Differences lie in their higher assumed intake of food for muscle work (with only ~2% overall efficiency), a lower mechanical drive efficiency (8% versus 11%) compared to that from our more granular ϵ -mpg empirical approach and a lower heat efficiency (7% versus 12%) as more heat is allocated to LTH in their analysis. Laitner's³⁹ subsequent 2000–2010 extension of their results estimated US efficiency to be 14% in 2010, higher than our static 11%. This is due to a much lower overall electricity efficiency in our analysis, resulting from the Carnot and granularity refinements noted above, coupled to the fact that electricity is a larger share of useful work by 2010. Reistad's² estimated 1970 US exergy efficiency of 22% is double our 11% value. This is because he estimated higher efficiencies for both transport (22% versus 13%, due to using significantly higher car/truck efficiencies versus other studies (e.g., ref 31)) and heating (20% versus 10%, based on much higher HTH operating temperatures and incorrectly omitting “first law” process efficiencies).

Warr et al.¹⁵ estimated UK exergy efficiency to rise from 8% to 14% from 1960 to 2000, which compares well to our results. The 1960 values are similar (8%) as their greater allocation of muscle work is offset by our lower electricity efficiency noted earlier. By 2000, our overall efficiency also matches theirs, as our lower efficiency values for heat (12% vs 17%) and electricity (14% vs 20%) are balanced by our higher efficiencies for mechanical drive (19% vs 14%) and our lower allocation of muscle work. Warr et al.'s earlier 2008 analysis¹⁹ estimated UK exergy efficiency rose from 10% (1960) to 15% (2000), similar to our values but the reasons for differences to their later results¹⁵ cannot be determined. Hammond and Stapleton's⁹ analysis for the UK does not include an overall exergy efficiency estimate, but their results for electricity, residential, industrial and transport sectors appear broadly similar to ours.

Differences between directly comparable exergy efficiency results (i.e., for same country and year) lie less in primary exergy (main differences exist in assumed food/muscle work inputs) and more in assumed task-level exergy efficiencies (e.g., LTH, MTH, HTH). Such differences to (and between) previous analysis results highlight the need for a common methodology, which is the goal to which this paper contributes. A consistent, comparable approach allows better understanding of energy consumption patterns and differences. But it also provides a solid analytical basis for exploration of extensions to energy services, linkages to economic growth, and informing future energy demand scenarios. For example, our analysis indicates that almost all of the useful work growth in the US has come from increasing primary exergy inputs, raising the question of the sustainability of this going forward. On the other hand, UK exergy efficiency improvements appear to be leveling off, raising the challenge of how to achieve further

efficiency improvements. This is important as Ayres and Warr argue that increases in primary exergy inputs and efficiency of conversion to useful work have been key drivers of economic growth in the US and UK.²⁵

Overall, the methodological framework and results in this paper have important implications that are the basis for suggested further studies. First, further standardization of the IEA-based calculation approach would be helpful, including consistent treatment of renewables, electricity end uses and nonenergy. For renewables, we follow previous exergy analyses (e.g., ref 19), which typically take solar and wind conversion device factors of 0.07–0.13, whereas the IEA assumes factors of 1.00. Second, evidence of efficiency dilution needs decomposition scrutiny, but if confirmed, it suggests aggregate exergy efficiency is no longer rising in either US or UK, despite implementing various energy efficiency measures in industry, residential and transport sectors, and this poses important questions. For example: does this indicate the UK (due to dilution) is close to a practical maximum for national energy efficiency? Or are higher efficiency processes “offshored” through exergy trade flow, in a similar way to carbon emissions?⁴⁰ Is dilution evidence of energy rebound (e.g., refs 41 and 42)? And if this exergy efficiency stagnation continues, would any future growth in useful work come wholly from primary exergy (energy) supply? Thus, both dilution and stagnation effects could have impacts on energy efficiency and energy supply policies.

Third, the links between exergy and economic growth are worthy of continued study. For example, studying the role of prices in the evolution of US–UK exergy efficiencies would add to existing econometric literature (e.g.²³), while the question of whether exergy efficiency stagnation would threaten the engine of economic growth²⁵ could be considered. Useful work intensity (useful work/GDP) may also offer additional insights into links between end energy use and efficiency, as Serrenho et al. propose,^{17,43} compared to traditional energy intensity (TPES/GDP) metrics, which some have criticized (e.g., refs 44 and 45). Fourth, the valuable extension of this technique to include research on energy services will help review practical and theoretical exergy efficiency limits, and be clearer on the delineation between active device and passive system efficiencies (e.g., ref 24). Last, is the effect on CO₂ reduction, because stagnation in exergy efficiencies result in closer coupling of energy and emissions, making it difficult to deliver on global mitigation objectives.

By considering end energy use from a quality viewpoint, exergy and useful work analysis appears well suited to examine current issues such as the use of lower grade fossil fuels, mainstreaming of renewables and future energy and economic forecasting. However, there are limits to a useful work second law approach: for example, exergy efficiency does not capture the effect of insulation/leak proofing on buildings except through reduced exergy inputs. For this, a passive system approach is required. Therefore, as Hammond and Stapleton⁹ suggest, exergy and useful work approaches should be seen as complementary and not competing with traditional (first law) energy analysis techniques.

■ ASSOCIATED CONTENT

📄 Supporting Information

Additional material, results and cited literature presented in three sections: S1, IEA mapping to useful work categories; S2,

detailed input data; S3, detailed outputs. This material is available free of charge via the Internet at <http://pubs.acs.org>.

AUTHOR INFORMATION

Corresponding Author

*Paul Brockway. E-mail: eepr@leeds.ac.uk.

Notes

The authors declare no competing financial interest.

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