Optimal Efficiency-Power Tradeoff for an Air Compressor/Expander
(1st Revision)

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Abstract

An efficient and power dense high pressure air compressor/expander is critical for the success of a compressed air energy storage (CAES) system. There is a trade-off between efficiency and power density that is mediated by heat transfer within the compression/expansion chamber. This paper considers the optimal control for the compression and expansion processes that provides the optimal trade-off between efficiency and power. Analytical Pareto optimal solutions are developed for the cases in which $hA$, the product of the heat transfer coefficient and heat transfer surface area, is either a constant or is a function of the air volume. It is found that the optimal trajectories take the form “fast-slow-fast” where the fast stages are adiabatic and the slow stage is either isothermal for the constant-$hA$ assumption, or a pseudo-isothermal (where the temperature depends on the instantaneous $hA$) for the volume-varying-$hA$ assumption. A case study shows that at 90% compression efficiency, power gains are in the range of 500 – 1500% over ad-hoc linear and sinusoidal profiles.

I. INTRODUCTION

Compressed air energy storage (CAES) is widely accepted as an economic grid scaled energy storage approach needed to meet the challenge of integrating more and more intermittent and variable renewable energy resources such as wind or solar into the electrical grid. A novel CAES system for off-shore wind turbines is proposed in [1]. For this and other CAES system, a critical component is the high pressure air compressor/expander (C/E) responsible for transforming energies between mechanical and pneumatic domains. To be effective, the C/E needs to be capable of high pressure (∼200bar), efficient, powerful enough to handle the power requirements, and compact enough so as to minimize capital cost and physical footprint. A C/E with these characteristics are also useful in other applications such as making liquefied gas or fueling vehicles powered by natural gas.

There is an inherent trade-off between efficiency and power density (power for a given size) that is a function of heat transfer. For example, as will be explained in section II, an isothermal process is the most efficient but requires a long cycle time for heat transfer to take place; adiabatic process can be infinitely fast, but is inefficient. A common hardware approach to improving this trade-off is to enhance heat transfer by adding extra thermal capacitances and heat transfer surface areas. Examples include elastomeric foams, [2], thin metal strands [3], and sprays of tiny water droplets [4], [5]. Our group’s approach is to use a liquid piston compressor/expander in conjunction with porous media inserts to increase the specific surface area for heat transfer while allowing free movement of the the piston which is the liquid/air interface [6], [7], [8], [9], [10].

In this paper, a software approach is proposed in which the compression and expansion trajectories are optimized and controlled to further improve performance. In the case of the liquid piston compressor/expander, arbitrary trajectories can be implemented simply by varying the liquid flow rates. Pareto optimal solutions are sought that optimize powers for given efficiencies or optimize efficiencies for given powers. In the literature, similar works are found in [11], [12], [13], [14], [15] where optimal control was derived using calculus of variation to maximize...
work output of heat engines. Here, we focus on air compressor/expanders and derive analytical solutions. Besides ideal gas assumption, it is assumed that the temperature of the heat source/sink is constant, and $hA$, the product of the heat transfer coefficient ($h$) and the heat transfer area $A$, is either a constant or a function of the air volume $V$. Although these assumptions are an idealization, these analytical solutions offer important insights into the problem of high pressure, efficient and powerful compressor/expanders. For specific problem with more general assumptions, numerical techniques such as parametric optimization and dynamic programming can be applied. See e.g. our more recent work [16], [17].

It is shown that the Pareto optimal compression/expansion trajectories take the form of consecutive fast-slow-fast segments. Specifically, in the constant $hA$ product case, the optimal trajectories are adiabatic-isothermal-adiabatic segment. In the volume dependent $hA(V)$ case, the isothermal sgement is replaced by a pseudo-isothermal section whose temperature depends on the instantaneous $hA$. The improvements can be quite significant. For example, in a CAES case study, the system is 5 – 15 times more powerful with optimized trajectories than with ad-hoc sinusoidal and linear trajectories! Preliminary results in this paper were presented in [18], [19] where only sketches of the proofs were provided.

The remainder of the paper is organized as follows: section II lays out the system model, assumptions, and definitions. Section III derives the optimal compression trajectory solution for the constant $hA$ case. Section IV extends the result to the volume varying $hA(V)$ case. Section V applies the solution to an energy storage scenario. Sections VI and VII discuss the results and offer some concluding remarks.

## II. SYSTEM MODEL AND PROBLEM STATEMENT

For the purposes of this paper, the air compressor/expander is assumed to be used in the open accumulator energy storage architecture in Fig. 1, although much of the analysis is generally applicable. The distinguishing feature of this configuration is that the compressed air pressure in the storage vessel can be maintained constant regardless of amount of compressed air present. This is accomplished by adjusting the liquid volume in the vessel which contains both liquid and compressed air.

To store energy, for every compression cycle, ambient air (assumed to be an ideal gas) at temperature and pressure, $T_0$ and $P_0$, is compressed to a temperature and pressure $T_c$ and $P_c$ inside the compression/expansion chamber according to a time-dependent pressure-volume trajectory: $\zeta_c(t) = (P(t), V(t))$. The compressed air is then ejected isobarically to the accumulator to be stored. Inside the accumulator, the compressed air is allowed to cool back to ambient temperature.

For energy regeneration, the compressed air is first injected from the accumulator into the compression/expansion chamber isobarically. The air then expands from $P_c$ and $T_0$ to the ambient pressure $P_0$ and and final temperature $T_e$ according to a pressure-volume trajectory $\zeta_e(t) = (P(t), V(t))$.

Work by the ambient pressure $P_0$ is subtracted out because it is assumed to be the case pressure of the compressor/expander. In accordance with the open accumulator concept, when compressed air is ejected into or injected from the storage vessel, an equivalent volume of liquid from the storage vessel is removed or added. Since the input/output work of the gas compressor/expander is retrieved/provided by the hydraulic pump/motor, the net
work associated with the ejection/injection process is zero. However, additional re-compression work is needed to maintain the compressed air pressure inside the accumulator as the compressed air is cooled.

The assumption that the air has time to return to equilibrium with the environment before expansion is compatible with applications that require storage on the order of hours or longer and is a conservative assumption in other cases.

The dynamics of the compression/expansion process are determined from the first law of thermodynamics and the equation of state for an ideal gas applied to the air within the compression/expansion chamber:

\[
nc_v \dot{T} = -P \dot{V} - q = -\frac{nRT}{V} \dot{V} - q
\]

\[
P = \frac{nRT}{V}
\]

(1)

where \(c_v = R/(\gamma - 1)\) is the constant volume specific heat of air on a molar basis, \(\gamma\) is the ratio of the specific heats, \((P,V,T)\) are the air pressure, volume, and temperature, \(n\) is the air quantity in moles, \(R\) is the universal gas constant, \(q\) is the heat transfer rate (out of the gas) described by

\[
q = hA(V)(T - T_0)
\]

(2)

where \(h\) is the heat transfer coefficient, \(A\) is the heat transfer surface area, and the heat sink/source temperature is assumed to be ambient \(T_0\). \(\dot{V}\), which determines the compression/expansion trajectory, can be considered the control input. In this paper, the \(hA\) product is assumed to be either a constant or a function of air volume only.

The assumption that air in the compressor/expander is an ideal gas is an idealization that is less accurate at higher pressures. In the case of the liquid piston compressor/expander, vaporization and condensation of the water also have thermodynamic effects (although, the effect is only appreciable at low efficiency operating regimes to increase power density but its effect is insignificant at high efficiency regimes [21]). However, in light of the simplified heat transfer model, the ideal gas model is reasonable to in order obtain analytical near closed form solutions. As mentioned earlier, more complex models can be investigated numerically such as for detailed designs.

The cycle compression work input \(W_{in}\) and expansion work output \(W_{out}\) are given by the shaded areas as shown in Fig. 2. These areas exclude the ejection and injection work but the compression work includes the isobaric

\[\text{For a standalone compressor/expander not in an open accumulator, } W_{in} \text{ and } W_{out} \text{ would include additional term } (P_c - P_0)V_s = nRT_0(1 - 1/\gamma). \text{ This has the effect of increasing the efficiency and power values. However, since the extra term is a constant, it does not affect the optimization process.}\]
cooling work in accordance with the open accumulator concept. The compression work input is:

$$W_{in}(\zeta_c) \equiv -\int_0^{t_c} (P(t) - P_0) \dot{V}(t) \, dt$$

\hspace{1cm} + nR \frac{1}{1/r} (T_c - T_0) \tag{3}$$

The expansion work output is:

$$W_{out}(\zeta_e) \equiv \int_0^{t_e} (P(t) - P_0) \dot{V}(t) \, dt$$

\hspace{1cm} = \frac{1}{nR} \frac{1}{1/r} (T_e - T_0) \tag{4}$$

Note that $W_{in} = W_{out}$ if $\zeta_c$ and $\zeta_e$ are isothermal processes at $T = T_0$. Hence, the work for isothermal compression or expansion is the maximum work available and is defined to be the stored energy for compressing this amount of gas to $P_c$. It is given by:

$$E \equiv nRT_0 \left[ \ln (r) - 1 + \frac{1}{r} \right]. \tag{5}$$

where $r := P_c/P_0 > 1$ is the pressure ratio.

Compression and expansion efficiencies are defined as:

$$\eta_c(\zeta_c) \equiv \frac{E}{W_{in}(\zeta_c)} \quad \text{and} \quad \eta_e(\zeta_e) \equiv \frac{W_{out}(\zeta_e)}{E}. \tag{6}$$

The rate at which energy is stored or regenerated is the power. Therefore compression and expansion powers are defined as

$$\text{Pow}_c(\zeta_c) \equiv \frac{E}{t_c} \quad \text{and} \quad \text{Pow}_e(\zeta_e) \equiv \frac{W_{out}(\zeta_e)}{t_e} \tag{7}$$

where $t_c$ and $t_e$ are the compression and expansion process times to execute trajectories $\zeta_c$ and $\zeta_e$. From the 1st law (1) and Newton’s law of cooling (2), $t_c$ and $t_e$ are:

$$t_{c/e} \equiv \int dt = \int \frac{qdt}{hA(V)(T - T_0)} = \int \frac{nc_e dT + PdV}{hA(V)(T - T_0)} \tag{8}$$

where $dT = (PdV + VdP)/nR$ and the integration is executed over the trajectories $\zeta_c(\cdot)$ and $\zeta_e(\cdot)$. Ejection to and injection from the storage vessel, fresh air intake from and expanded air exhaust to the low pressure buffer (or atmosphere) are assumed to take no time as they are not limited by heat transfer. Therefore the power defined in (7) can be considered thermodynamic limited power. The actual power will be lower due to the finite time needed for these non-thermodynamic limited processes.

There is a inherent conflict between efficiency and power. For example, isothermal compression/expansion at $T = T_0$ are 100% efficient but from (8), the process times are infinite, resulting in zero power. On the other hand, adiabatic processes take zero times (hence high power) but, as illustrated, Fig. 2, the energy loss is large so that efficiencies are low. Note from (8) that the numerator determines the P-V curve and hence, efficiency, whereas increasing the denominator decreases process time and increases power. Thus, increasing the heat transfer capability given by $hA(V)$ can increase power without sacrificing efficiency. In this paper, we go further by utilizing optimal control to make the best use of the available heat transfer capability.

**Problem statement:** To determine Pareto optimal trajectories $\zeta_c^\ast(t)$ for compression from $(P_0, T_0)$ to $P_c$ with subsequent isobaric cooling, and $\zeta_e^\ast(t)$ for expansion from $(P_c, T_0)$ to $P_0$, such that: for a given efficiency, no other trajectory provides more input power $W_{in}$ or output power $W_{out}$ than the Pareto optimal trajectory; for a given power, no other trajectory operates at higher efficiency than the Pareto optimal trajectory. The optimization problem is expressed as

$$\max_{\zeta} \text{Pow}_{c/e}(\zeta) \quad \text{s.t.} \quad \eta_{c/e}(\zeta) = \eta^\ast \tag{9}$$

where $\eta^\ast$ is some prescribed efficiency. Or equivalently,

$$\max_{\zeta} \eta_{c/e}(\zeta) \quad \text{s.t.} \quad \text{Pow}_{c/e}(\zeta) = \text{Pow}^\ast \tag{10}$$

where Pow$^\ast$ is some prescribed power. In (9), (10), $\eta_{c/e}$ and Pow$_{c/e}$ are defined in (6) and (7) respectively.
Remark 1. In the optimization procedures below, we solve the problem of minimizing process times $t_c$ or $t_e$ while constraining input work $W_{in}$ or output $W_{out}$ (or optimizing $W_{in}$ or $W_{out}$ while prescribing process times). It will be shown in Remark 2 that it is equivalent to maximizing power while prescribing efficiency (or maximizing efficiency while prescribing power).

III. CONSTANT $hA$ OPTIMAL TRAJECTORIES

In this section, we derive the Pareto optimal compression/expansion trajectories for the case when the $hA$ product in (2) is a positive constant and the heat sink/source is at temperature $T_0$. Instead of optimizing with respect to efficiency and power, we optimize with respect to input/output work and process time instead.

The derivation proceeds in these two steps:
Step 1: A physically feasible process $\zeta$ between two arbitrary endpoints $(P_0, V_0)$ and $(P_f, V_f)$ can be improved with an $A-I-A$ process $\zeta^*$ between the same endpoints consisting of an adiabatic (A) process, an isothermal (I) process, and a final adiabatic (A) process. The work associated with the AIA process is the same but the process time will be the same or reduced.

Step 2: For the given initial $(P_0, V_0)$, final pressure $P_f$, and for each prescribed efficiency, the final volume $V_f$ and the isothermal temperature $T^*$ of the AIA process are optimized to minimize the process time while matching the prescribed efficiency (or to optimize work while matching the prescribed process time).

Step 1 is further divided into two sub-steps. Let $\zeta$ be a process between two arbitrary endpoints $(P_0, V_0)$ and $(P_f, V_f)$ that is physically feasible with heat transfer with the heat source/sink at the temperature $T_0$. Since any such process can be uniformly approximated by a sequence of isothermal (I) and adiabatic (A) processes, without loss of generality, $\zeta$ is assumed to consists of such alternate I and A process steps as illustrated in Fig. 3. In step 1A, we show that an isothermal-adiabatic-isothermal (IAI) isothermal (IAI) sub-sequence can be replaced by an adiabatic-isothermal-adiabatic (AIA) sub-sequence with reduced process time but equal work. Then, in step 1B, this procedure is propagated through the entire original process $\zeta$ to form a global AIA replacement sequence with equal work and reduced process time.

A. Step 1A: Improving IAI process time with AIA process.

Consider an IAI sub-sequence of the original process curve $\zeta$ that has been approximated by alternate A and I steps (Fig. 3). Suppose that the IAI sub-sequence traverses through states A-B-C-D where A-B and C-D are isothermal steps at temperatures $T_A$ and $T_D$, and B-C is an adiabatic step.

The boundary work done ($W = \int PdV$) on the gas is:

$$W_{IAI} = W_{AB} + W_{BC} + W_{CD}$$

$$= nR \left[ T_A \ln(P_B/P_A) + \frac{(T_D - T_A)}{\gamma - 1} + T_D \ln(P_D/P_C) \right]$$

(11)
Since the adiabatic step takes no time, the process time is:

\[ t_{IAI} = \frac{nR}{hA} \left[ \frac{T_A \ln(P_B/P_A)}{T_A - T_0} + \frac{T_D \ln(P_D/P_C)}{T_D - T_0} \right] \]  

(12)

To be physically feasible, each term should be positive.

Consider now an alternate AIA sequence that traverses the states A-E-F-D where A-E and F-D are adiabatic steps and E-F is isothermal at temperature \( T_E \). The work on this alternate sequence is:

\[ W_{AIA} = W_{AE} + W_{EF} + W_{FD} \]

\[ = nR \left[ \frac{(T_D - T_A)}{\gamma - 1} + T_E \ln(P_F/P_E) \right] + T_D \ln(P_D/P_C) \]

(13)

Note that the total adiabatic works are the same for the two sequences since the temperature changes are the same. The process time becomes:

\[ t_{AIA} = \frac{nR}{hA} \left[ \frac{T_E \ln(P_F/P_E)}{T_E - T_0} \right] \]

(14)

which must be positive to be physically feasible.

It can be shown that the products of the isothermal pressure ratios are the same for the two sequences:

\[ P_B/P_A \cdot P_D/P_C = P_F/P_E : = r_I \]

(15)

Thus, we can write for some \( x \in \mathbb{R} \)

\[ P_B/P_A = r_I^x, \quad P_D/P_C = r_I^{1-x}. \]

If the temperature \( T_E \) is chosen such that the work \( W_{AIA} \) by A-E-F-D (AIA) is the same as the work \( W_{IAI} \) by A-B-C-D (IAI), then utilizing (15) and comparing (11) and (13), \( T_E \) must be:

\[ T_E = xT_A + (1-x)T_D \]

(16)

Let \( \Delta s \) be the time difference normalized by the AIA time:

\[ \Delta s := \frac{t_{IAI} - t_{AIA}}{t_{AIA}}. \]

(17)

Thus, \( \Delta s > 0 \) would signify a decrease in process time by the AIA sequence. Utilizing (15) and (16) and some algebra, the normalized time difference can be written as:

\[ \Delta s = \frac{T_0}{T_E} \left[ \frac{x(T_E - T_A)(T_D - T_A)}{(T_A - T_0)(T_D - T_0)} \right] \]

(18)

To evaluate the sign of \( \Delta s \), we consider the following cases to determine the sign of the terms inside \([\cdot]\) in (18).

**Case 1:** \( r_I > 1, \ 0 < x < 1. \)

In this case, \( T_A > T_0 \) and \( T_D > T_0 \) (in order for each term in (12) to be positive). From (16), \( T_E \) is between \( T_A \) and \( T_D \).

**Case 2:** \( r_I > 1, \ x < 0. \)

In this case, \( T_A < T_0 < T_D \) (for each term in (12) to be positive). Combined this with (16), we have \( T_A < T_D < T_E \).

**Case 3:** \( r_I > 1, \ 1 < x. \)

In this case, \( T_D < T_0 < T_A \) (for each term in (12) to be positive). Combined this with (16), we have \( T_D < T_A < T_E \).

**Case 4:** \( r_I < 1, \ 0 < x < 1. \)

In this case, \( T_A < T_0 \) and \( T_D < T_0 \) (in order for each term in (12) to be positive). From (16), \( T_E \) is between \( T_A \) and \( T_D \).

**Case 5:** \( r_I < 1, \ x < 0. \)

In this case, \( T_D < T_0 < T_A \) (for each term in (12) to be positive). Combined this with (16), we have \( T_E < T_D < T_A \).

**Case 6:** \( r_I < 1, \ 1 < x. \)

In this case, \( T_A < T_0 < T_D \) (for each term in (12) to be positive). Combined this with (16), we have \( T_E < T_A < T_D \).
Let the AIA process goes through points $r_I$, $r_F$, and $r_D$. For the boundary case of $r_I > 1$, AIA collapses to a single adiabatic step so that $t_{AIA} = 0$. It would be smaller than the finite $t_{IAI}$ except when $P_B/P_A = D/P_C = 1$ where the IAI also collapses to a single adiabatic step. If $x = 0$ or $x = 1$, one of the $I$'s in the original IAI collapses to a point. They can already be considered an AIA with a trivial $A$. Thus, process time is not affected.

The overall effect is that in all cases, $\Delta s \geq 0$ while only when $P_B/P_A = 1$ or $D/P_C = 1$, $\Delta s = 0$.

**B. Step 1B: Improving process time of whole process by a global AIA process**

Step 1A above shows that a physically feasible IAI process can be replaced by a AIA process with the same endpoints and same boundary work but shorter process time. The procedure can be propagated to attain a global AIA process that improves upon an arbitrary physically feasible process with the same endpoints and same work but shorter process time.

To see this, suppose that the original process $\zeta$ is adequately approximated by the sequence of isothermal and adiabatic segments:

$$\begin{align*}
I_1A_1I_2A_2I_3 \ldots A_kI_k \ldots
\end{align*}$$

Replacing $I_1A_1I_2$ by $A'_1I'_1A'_2$ with the same work but reduced time, we have

$$A'_1I'_1A'_2A_2I_3 \ldots A_kI_k \ldots$$

Since $A'_2A_2 = A''_2$ is together a single adiabatic, we have a sequence with fewer segments,

$$A'_1I'_1A''_2I_3 \ldots A_kI_k \ldots$$

The process can be continued by iteratively replacing an IAI sequence by an AIA, and combining the resulting consecutive $A$'s into a single $A$ segment. As the number of segments reduces, eventually, the replacement sequence becomes a 3-segment AIA. The two end points and the boundary work for the final AIA are unchanged but the process time is reduced. The result for step 1 is summarized as follows.

**Proposition 1.** Given an initial and final points $(P_0, V_0)$ and $(P_f, V_f)$, the process with the least process time $t$ that provides the prescribed feasible boundary work $W = \int_0^t P \, dV$ consists of a sequence of adiabatic-isothermal-adiabatic (AIA) segments.

**Proof.** The proof is simply that any feasible candidate process that provides the prescribed work can be subjected to the improvement process above unless it itself is an AIA process.

**C. Step 2: Optimizing the AIA trajectory**

In this step, the AIA trajectory is optimized to minimize the process time. We first focus on the compression process. It is assumed that the initial $(P_0, V_0, T_0)$ and the final $P_c = rP_0$ are given and the work input is prescribed. Note the molarity $n = (P_0V_0)/(RT_0)$.

Let the AIA process goes through points $(P_i, V_i, T_i)$ for $i = 0, 1, 2, 3$ with $P_3 = P_c$ and $T_1 = T_2$. Steps 0–1 and 2–3 are adiabatic steps and step 1–2 is isothermal. The process can be uniquely parametrized by temperatures $(T_1, T_c)$. Therefore, using the property of the adiabatic process,

$$\begin{align*}
\left( \frac{P_1}{P_0} \right)^\frac{\gamma-1}{\gamma} &= \frac{T_1}{T_0}, & \left( \frac{P_c}{P_2} \right)^\frac{\gamma-1}{\gamma} &= \frac{T_c}{T_1}
\end{align*}$$

- **Note the molarity process.** It is assumed that the initial process is adiabatic (AIA) segments.

- **Proof.**

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$$\begin{align*}
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\end{align*}$$
so that the isothermal pressure ratio is:

\[ r_I := \frac{P_2}{P_1} = r \left( \frac{T_c}{T_0} \right)^{-\frac{\gamma}{\gamma-1}} \]

The prescribed work in terms of \( T_1, T_c \) is therefore:

\[
W_{in}(T_1, T_c) = nR \left\{ T_1 \left[ \ln(r) - \frac{\gamma}{\gamma-1} \ln \left( \frac{T_c}{T_0} \right) \right] + \frac{\gamma}{\gamma-1} (T_c - T_0) - T_0(r - 1)/r \right\}
\]

The process time is:

\[
t_e(T_1, T_c) = \frac{nR}{hA} \left( \frac{T_1}{T_1 - T_0} \right) \left[ \ln(r) - \frac{\gamma}{\gamma-1} \ln \left( \frac{T_c}{T_0} \right) \right]
\]

The constrained minimization problem with prescribed work input \( W^\dagger \) can be formulated as an unconstrained optimization using Lagrange multiplier:

\[
\min_{T_1, T_c, \lambda} t_e(T_1, T_c) + \lambda (W_{in}(T_1, T_c) - W^\dagger)
\]

so that the first order extremum conditions are:

\[
\begin{align*}
\frac{\partial t_e}{\partial T_1} + \lambda \frac{\partial W_{in}}{\partial T_1} &= 0 \\
\frac{\partial t_e}{\partial T_c} + \lambda \frac{\partial W_{in}}{\partial T_c} &= 0
\end{align*}
\]

Solving for and equating \( \lambda \) from each expression yields:

\[
\lambda = \frac{T_0}{T_1 - T_0} = \frac{T_1}{(T_1 - T_0)(T_c - T_1)}
\]

\[ \Rightarrow \quad T_1 = \sqrt{T_0 \cdot T_c} \] (22)

This establishes the relationship between the isothermal temperature of the AIA trajectory and the initial and final temperatures. Different choices of \( T_1 \) (or \( T_c \)) result in different work input.

A similar procedure can be applied to minimize the work input while satisfying a prescribed time. This results in the same relation (with \( \lambda \) replaced by \( 1/\lambda \) in (21)) between \( T_0, T_1 \) and \( T_e \) in (22).

For the expansion case, we specify the initial \((rP_0, V_s, T_0)\) and the final pressure \( P_0 \). The AIA is parametrized by the isothermal temperature \( T_1 \) and final temperature \( T_e \). The output work and expansion time are given instead by:

\[
W_{out}(T_1, T_e) = nR \left\{ T_1 \left[ \ln(r) - \frac{\gamma}{\gamma-1} \ln \left( \frac{T_0}{T_e} \right) \right] + \frac{\gamma}{\gamma-1} (T_0 - T_e) - T_0(1 - 1/r) \right\}
\]

\[
t_e(T_1, T_e) = \frac{nR}{hA} \left( \frac{T_1}{T_0 - T_1} \right) \left[ \ln(r) - \frac{\gamma}{\gamma-1} \ln \left( \frac{T_0}{T_e} \right) \right]
\]

The optimal trajectory can be found by optimizing the time while matching the prescribed work output, or optimizing work output while matching the prescribed time. Both result in the same expression:

\[ T_1 = \sqrt{T_0 \cdot T_e} \] (25)

Note that since optimizing time while prescribing work, and optimizing time while prescribing time give the same trajectories, the optimal trajectories are the Pareto optimal.

We summarize the results for the constant \( hA \) case in the following theorem.

**Theorem 1.** Let \( P_0 \) and \( T_0 \) be the ambient pressure and temperature. Assume an ideal gas model, and in (2), the heat transfer coefficient-area product \( hA \) is constant and the heat sink/source is at \( T_0 \).
(Compression) The trajectory \( \zeta_c^* \) that compresses the gas from \((P_0, T_0)\) to a pressure of \( rP_0 \) with \( r > 1 \) consisting of an instantaneous adiabatic compression from \((P_0, T_0)\), followed by an isothermal compression at \( T_{iso} \), and finally followed by another instantaneous adiabatic compression to the desired pressure \( rP_0 \) and the final temperature of \( T_c \) such that:

\[
T_{iso} = \sqrt{T_0 \cdot T_c}
\]

is a Pareto optimal trajectory with respect to minimizing input work \( W_{in} \) given by (3) and compression time \( t_c \) given by (8).

(Expansion) The trajectory, \( \zeta_e^* \) that expands the gas from \((rP_0, T_0)\) to \( P_0 \) with \( r > 1 \) consisting of initial and final instantaneous adiabatic stages and an intermediate isothermal stage where the isothermal stage temperature \( T_{iso} \) and final temperature \( T_e \) are related by:

\[
T_{iso} = \sqrt{T_0 \cdot T_e}
\]

is a Pareto optimal with respect to maximizing output work (4) and minimizing process time (8).

For both compression and expansion, the Pareto frontier is generated by the choosing different \( T_{iso} \) (or final temperatures \( T_c \) or \( T_e \)).

Remark 2. Although Theorem 1 is stated in terms of input/output work (3)-(4) and process time (8), the same trajectories are optimal with respect to efficiencies (6) and powers (7). It is so because prescribing efficiency is equivalent to prescribing input/output work. Also, for compression, maximizing power is equivalent to minimizing process time. For expansion, the first order optimality condition for maximizing power with the prescribed work output using the Lagrange multiplier is, in place of (21), given by:

\[
\frac{\partial Pow_e}{\partial \theta} + \lambda \frac{\partial \eta_e}{\partial \theta} = 0
\]

\[
\Rightarrow \left( \lambda + \frac{1}{t} \right) \frac{\partial W_{out}}{\partial \theta} - \frac{W_{out}}{t^2} \frac{\partial t_e}{\partial \theta} = 0
\]

for \( \theta = t_e \) and \( T_1 \). Thus, solving for and equating \( t(t\lambda + 1)/W_{out} \) for each \( \theta \) gives the same condition as for the case of minimizing expansion time with a constraint in output work.

IV. Volume Dependent \( hA \) Optimal Trajectory

In this section, we extend the result in section III to the case when the heat transfer coefficient-area product \( hA(V) \) in (2) is a differentiable function of the gas volume \( V \). This will be especially important with a liquid piston compressor/expander with the chamber being filled with porous media so that the heat transfer area will decrease as the chamber volume decreases. The solution is derived in two steps:

Step 1: We will first show that Pareto optimal monotonic compression or expansion trajectories must consist of segments of two adiabatic (A) segments sandwiching a pseudo-isothermal (pI) segment (i.e. ApIA). Instead of being at a constant temperature as in the constant \( hA \) case, the temperature within the pseudo-isothermal segment varies with the \( hA \) for the instantaneous volume.

Step 2: The parameters for the ApIA trajectory will be optimized to minimize the process time for the prescribed work (or equivalently, to optimize work for the prescribed process time).

A. Step 1: Optimal trajectories consist of Adiabatic (A), pseudo-Isothermal (pI), and Adiabatic (A) segments

We discretize the differentiable \( hA(V) \) function into \( N \) (which will be taken to be \( \infty \)) constant \( hA \) segments such that: for \( i = 1, 2, \ldots, N \),

\[
hA(V) = (hA)_i \quad \text{for } V_{i-1} \geq V > V_i
\]

Here, \( V_N < V_{N-1} < \ldots < V_1 < V_0 \) represent the transition volumes at which the \( hA \) product changes to a new value. From Proposition 1, over each constant \( hA \) volume interval \((V_i, V_{i-1})\) and for given initial and final pressures and volumes, the optimal trajectory with respect to work and time takes the form of an adiabatic-isothermal-adiabatic (AIA) trajectory.
Consider consecutive constant $hA$ intervals $(V_i, V_{i-1})$ for $i = 1, \ldots, N$. Let the isothermal temperatures be $T_{i-1}^{iso}$ for the interval $(V_i, V_{i-1})$ and the temperature at $V_i$ be $T_i$ for each $i$ (see Fig. 4).

The boundary work ($\int PdV$) over these $N$ segments is:

$$W = \frac{nR(T_N - T_0)}{\gamma - 1} + \sum_{j=1}^{N} \frac{nRT_j^{iso}}{\gamma - 1} \ln \left[ \frac{T_{j-1}V_{j-1}^{\gamma-1}}{T_jV_j^{\gamma-1}} \right]$$

and the process time over these $N$ segments is:

$$t = \sum_{j=1}^{N} \frac{nRT_j^{iso}}{T_jV_j^{\gamma-1}} \ln \left[ \frac{T_{j-1}V_{j-1}^{\gamma-1}}{T_jV_j^{\gamma-1}} \right]$$

Using the Lagrange multiplier method to optimize $t$ (or $W$) while constraining $W$ (or $t$), the 1st order optimality condition gives: for $\theta = T_i^{iso}, T_i$ for each $i = 1, \ldots, N$,

$$\lambda \frac{\partial W}{\partial \theta} = -\frac{\partial t}{\partial \theta}$$

where $\lambda$ is the Lagrange multiplier common for all $\theta$. Derivatives w.r.t. $T_i^{iso}$ for different $i$ give:

$$\left[ \lambda - \frac{T_0}{hA_i(T_i^{iso} - T_0)^2} \right] \ln \left[ \frac{T_{i-1}V_{i-1}^{\gamma-1}}{T_iV_i^{\gamma-1}} \right] = 0$$

This implies each segment is either an entire adiabatic ($T_{i-1}V_{i-1}^{\gamma-1} = T_iV_i^{\gamma-1}$) or $T_0/\lambda = hA_i(T_i^{iso} - T_0)^2$. Derivative w.r.t. to $T_i$ gives information in regard to the transition temperature $T_i$ (see [10] for details). However, this information is not useful as we take $N \to \infty$.

Since $hA(V)$ is a differentiable function, as $N \to \infty$, $|hA_i - hA_{i+1}| \to 0$. Hence, two consecutive isothermal temperatures, $T_i^{iso}$ and $T_{i+1}^{iso}$, become infinitesimally close and the adiabatic portion (of the AIA for each constant $hA$ interval) that transitions between the two isotherms also vanishes. This means that as $N \to \infty$, contiguous non-adiabatic intervals form intervals where the temperature is given by:

$$\frac{T_0}{\lambda} = hA(V)(T(V) - T_0)^2$$

with $\lambda > 0$ being the parametrization. The segments in (31) are referred to as pseudo-isothermal (pI) segment since it reduces to an isotherm when $hA(V)$ is a constant.
Fig. 5. Replacing the pl-A-pl trajectory A-B-C-D by the pl-A trajectory A-E-D reduces work input (shaded area), and eliminates time to execute E-B and C-D.

Note that for each $\lambda > 0$ in (31), there are two possible solution branches: $T(V) - T_0 > 0$ or $T(V) - T_0 < 0$. The appropriate branch must be consistent with the direction of heat transfer according to (1)-(2) by checking the sign consistency in:

$$nR \left( \frac{T'_{pl}}{\gamma - 1} + \frac{T_{pl}}{V} \right) \dot{V} = -hA(V)(T_{pl}(V) - T_0)$$

where the superscript $'$ denotes derivative w.r.t. $V$ and

$$T'_{pl} = \pm \frac{1}{2} \sqrt{\frac{T_0}{\gamma hA V hA}}$$

with the $-/+$ signs corresponding to $T > T_0$ and $T < T_0$ respectively. For the compression process, $(T - T_0) > 0$ is the nominal branch with decreasing volume. For the expansion process, $(T - T_0) < 0$ is the nominal branch with increasing volume. Also when $hA(V)$ increases monotonically with $V$ (as is expected in practical applications), only the nominal branch is feasible.

Beside the pseudo-isothermal segments, from (30), adiabatic segments can also exist. However, they can only exist at the beginning or end of the trajectories, or as transitions between the two feasible pseudo-isothermal branches of (31). It is because two points on the same branch of a feasible pl (31) cannot be connected by an adiabatic as transversing the pl involves continuous heat transfer in one direction whereas traversing the adiabatic involves no heat transfer.

For the practical case where $\partial hA/\partial V \geq 0$, it is easy to see from Fig. 5 that a pl-A-pl trajectory where the two pl’s correspond to two branches (and different volume directions) is less efficient and takes more time than a direct pl-A or A-pl. Thus, trajectories with interior A segments are not optimal in this case. For more generic $hA(V)$ functions, by restricting volume trajectory $V(t)$ to be non-increasing for compression; and non-decreasing for expansion, then only the nominal branch of the pl is possible$^2$.

The above discussion leads to the following result:

**Proposition 2.** If $hA(V)$ is is a non-decreasing differentiable function of $V$ or the volume trajectory is restricted to be monotonic, the Pareto optimal trajectory must be an ApIA trajectory consisting of two adiabatic (A) segments sandwiching a pseudo-isothermal (pl) segment.

### B. Step 2: Optimizing the ApIA trajectory

We assume that either $hA'(V) \geq 0$ or the volume trajectory is restricted to be monotonic so that Proposition 2 holds. In this step, the ApIA trajectory is optimized to minimize the process time $t_{c/e}$ in (8) for a prescribed $W_{in}$

$^2$as adiabatic transition to the non-nominal branch must involve a reversal of volume change direction. For example, in a compression process to reach the branch with $(T - T_0) < 0$ either from an initial temperature of $T_0$ or from a branch with $(T - T_0) > 0$, the transition adiabatic segment must increase volume to reduce temperature. Similar argument applies for compression.
Fig. 6. Optimal compression for a continuously varying $hA$ product consists of three stages: adiabatic compression; $hA$-dependent compression; adiabatic compression. The slow $hA$-dependent curve is determined by the parameter $\lambda_c$. After the air is moved to the accumulator, the air volume is further reduced by isobaric cooling.

in (3) or $W_{out}$ in (4). For compression, the initial $(P_0, V_0, T_0)$ and the final $P_c = rP_0$ are given. For expansion, the initial $(rP_0, V_s, T_0)$ and the final pressure and volume $P_0$ are given.

Each ApIA trajectory is uniquely specified by the volume $V_a$ at which the first $A$ transitions to the pl, and the volume $V_b$ at which the pl transitions to the final $A$. It can also be specified by the Lagrange multiplier $\lambda$ in (31) (implicitly defined by $V_a$), and the final temperature $T_c$ (for compression) or $T_e$ (for expansion). Let $T_a$ and $T_b$ be the temperatures at $V_a$ and $V_b$.

For compression, the pl segment is characterized by

$$T_{pl}(V) = T_0 + \sqrt{\frac{T_0}{\lambda \cdot hA(V)}}$$

The input work $W_{in}$ is:

$$\frac{W_{in}}{nR} = \frac{(T_a - T_0) + (T_c - T_b)}{\gamma - 1} - \frac{\int_{V_a}^{V_b} T_{pl}(V) \frac{dV}{V}}{nR} + \frac{rP_0}{nR} \left( V_c - \frac{V_0}{r} \right) - \frac{P_0V_0}{nR} \left( 1 - \frac{1}{r} \right)
+ \frac{\gamma(T_c - T_b)}{\gamma - 1} - \frac{T_0 - T_a}{\gamma - 1} + T_0 \ln \left( \frac{V_a}{V_b} \right)
- \frac{T_0}{\lambda} \int_{V_a}^{V_b} \frac{dV}{V\sqrt{hA(V)}} - T_0 \left( 1 - \frac{1}{r} \right)$$

From (1), along a pseudo-isothermal,

$$-nR \left( \frac{T_{pl}'}{\gamma - 1} + \frac{T_{pl}}{V} \right) dV = hA(V)(T_{pl}(V) - T_0)dt$$
where $T_{pl}' = \partial T_{pl}/\partial V$ so that the process time $t_c$ is:

$$
\frac{t_c}{nR} = - \int_{V_a}^{V_b} \frac{G(\lambda, V)}{hA(V)(T_{pl}(V) - T_0)} dV
$$

$$
= - \int_{V_a}^{V_b} \frac{dV}{VhA(V)} - \sqrt{T_0\lambda} \int_{V_a}^{V_b} \frac{dV}{V\sqrt{hA(V)}}
+ \frac{1}{2(\gamma - 1)} \left[ \frac{1}{hA(V_a)} - \frac{1}{hA(V_b)} \right].
$$

(34)

As before, the adiabatic stages are instantaneous and do not contribute to the compression time. In the above $\lambda, T_a, T_b, T_c$ are related to $V_a$ and $V_b$ by:

$$
T_a = \left( \frac{V_0}{V_a} \right)^{\frac{1}{r}} T_0
$$

(35)

$$
\lambda = \frac{T_0}{hA(V_a)(T_a - T_0)^2}
$$

(36)

$$
T_b = T_0 + \sqrt{\frac{hA(V_a)}{hA(V_b)}} (T_a - T_0)
$$

(37)

$$
T_c = \left( \frac{V_b}{V_b} \right)^{\frac{1}{r}} T_0^{\frac{1}{r}}
$$

(38)

Using the same technique as in the constant $hA$ case to equate the Lagrange multiplier while constraining $W_{in}$ (or $t_c$) and optimizing $t_c$ (or $W_{in}$), the optimality condition is obtained as (using $V_a$ and $V_b$ as independent variables)

$$
\frac{\partial t_c}{\partial V_a} \frac{\partial W_{in}}{\partial V_b} = \frac{\partial t_c}{\partial V_b} \frac{\partial W_{in}}{\partial V_a}
$$

(39)

Eq. (39) and the constraint $t_c = t_c^*$ (or $W_{in} = W_{in}^*$), together with the dependent variables in (35)-(38), form a system of two equations and two unknowns which may be solved for the optimal $V_a$ and $V_b$. A combination of symbolic and numerical analysis can be used. The Pareto frontier can be generated by evaluating $W_{in}$ and $t$ for all solutions $(V_a, V_b)$ that satisfy (39).

The expansion case is similar, with the pseudo-isothermal given by:

$$
T_{pl}(V) = T_0 - \sqrt{\frac{T_0}{\lambda \cdot hA(V)}}
$$

(40)

The output work $W_{out}$ (4) and process time $t_e$ given by:

$$
W_{out} = \gamma \left( \frac{T_0 - T_e}{\gamma - 1} \right) - \frac{T_a - T_b}{\gamma - 1} + T_0 \ln \left( \frac{V_b}{V_a} \right)
- \sqrt{\frac{T_0}{\lambda}} \int_{V_a}^{V_b} \frac{dV}{V\sqrt{hA(V)}} - T_0 \left( 1 - \frac{1}{r} \right)
$$

(41)

$$
\frac{t_e}{nR} = - \int_{V_a}^{V_b} \frac{dV}{VhA(V)} + \sqrt{T_0\lambda} \int_{V_a}^{V_b} \frac{dV}{V\sqrt{hA(V)}}
+ \frac{1}{2(\gamma - 1)} \left[ \frac{1}{hA(V_a)} - \frac{1}{hA(V_b)} \right].
$$

(42)

The optimality condition is:

$$
\frac{\partial t_e}{\partial V_a} \frac{\partial W_{out}}{\partial V_b} = \frac{\partial t_e}{\partial V_b} \frac{\partial W_{out}}{\partial V_a}.
$$

(43)

**Theorem 2.** Let the product of the heat transfer coefficient and heat transfer area in (2) be a differentiable function $hA(V)$ of $V$. Suppose that either $hA(V)$ is monotonically increasing or the volume trajectory is restricted to be monotonic.
(Compression) The Pareto optimal volume trajectory that compresses a gas from \((P_0, T_0)\) to \(rP_0\) with respect to the input work \(W_{in}\) in (3) and process time \(t_c\) in (8) consists of an initial adiabatic portion, followed by a pseudo-isothermal portion given by (31), and ending with a final adiabatic portion. The transition points and the choice of the pseudo-isothermal curve satisfy (39).

(Expansion) The Pareto optimal volume trajectory that expands a gas from \((rP, T_0)\) to \(P_0\) with respect to the output work \(W_{out}\) in (4) and process time \(t_e\) in (8) consists of an initial adiabatic portion, followed by a pseudo-isothermal portion given by (40), and ending with a final adiabatic portion. The transition points and the choice of the pseudo-isothermal curve satisfy (43).

Following the same argument as in Remark 2, the trajectories given in Theorem 2 are also optimal with respect to efficiencies (6) and powers (7).

V. CASE STUDY

In this case study, we consider a compressed air energy storage (CAES) application for a wind turbine. A simplified system is shown in Fig. 7 in which a liquid piston compressor/expander (C/E) is connected to the mechanical shaft of the wind turbine-electric generator.

The chamber of the C/E is a 12 m\(^3\) cylindrical drum, with an aspect ratio of unity. To increase the heat transfer area, it is filled uniformly with a perfectly conducting metallic wire mesh bonded to the isothermal chamber walls. Excess wind energy is used to power the water pump/motor that pumps water to fill the chamber, compressing the air above the water piston. To regenerate energy, compressed air is expanded causing the water piston to retreat and to motor the pump/motor to power the generator. As the water fills the chamber, the porous mesh becomes submerged and the surface area in contact with the air is reduced. The heat transfer coefficient \(h\) is assumed to be 100 W/m\(^2\)-K (a constant). Therefore, the \(hA\) product increases with air volume \(V\) affinely as

\[
hA(V) = h \left[ \frac{4V(1-\epsilon)}{\epsilon} + \frac{4V}{\epsilon D} + \frac{\pi D^2}{2} \right]
\]

where \(\epsilon = 99.5\%\) is the mesh porosity, \(d = 80\mu m\) is the diameter of a strand of mesh, \(D = 2.48m\) is the chamber diameter, and \(V\) is the instantaneous air volume. The temperature of the wire mesh is assumed to be constant at \(T_0 = 298K\). The pressure compression ratio is \(r = 350\) and the nominal power of the CAES system is 1 MW.

The optimal trade-off between compression efficiency (6) and storage power (7) using optimized AplA trajectories is shown in Fig. 8. As comparisons, trade-offs using sub-optimal (since \(hA\) is not a constant) AIA trajectories, sinusoidal and linear trajectories are also plotted. Sinusoidal and linear profiles are included as they are commonly generated using a reciprocating crank-slider and a constant speed piston respectively. For each type of trajectory, a trade-off exists in that efficiency decreases as power increases. At any efficiency, the optimal AplA trajectory has higher power than any other trajectory. For example, at 90% efficiency, the optimal AplA trajectory is 60% more powerful than the AIA solution, 500% more powerful than sinusoidal compression and over 1500% more powerful than linear compression. Correspondingly, for a given power requirement, the chamber of the compressor that uses the optimal trajectory can be 5 times more compact than the one that uses a sinusoidal profile. At the nominal power of 1MW, the AplA trajectory achieves an efficiency of 80.3% whereas the efficiencies of all other trajectories are in the range of 60 – 65%.
Figure 9 compares the various types of volume trajectories normalized by the total process time for two different efficiencies: 90% and 60%. As expected, the sub-optimal AIA and the optimal ApIA both have a instantaneous stage, a slow stage, and a final instantaneous stage. The ApIA’s have shorter adiabatic portions than AIAs. Also, higher efficiency trajectories have shorter adiabatic compression stages.

The expansion efficiency versus power output trade-off is shown in Fig.10. Similar to compression, the optimal ApIA has the highest efficiency for given power and the highest power for a given efficiency.

As an example, the transition temperatures and metrics for the optimal ApIA trajectory at the nominal 1MW power are shown in Tab. II.

VI. DISCUSSION

It has been assumed that the adiabatic portion of the compression/expansion process takes zero time. In real situations, there are physical limitations to the compression and expansion rates so truly adiabatic processes are not possible. This effect is investigated for the case when $h_A$ is a constant, i.e. the optimal trajectories are AIA.

Let the compression rate be limited by $\dot{V}_{max}$ and define $p$ to be the ratio of $\dot{V}_{max}$ to the maximum compression rate during the isothermal sections. Since $\dot{V}_{max}$ is finite, finite time is needed to traverse volume change during the adiabatic sections, decreasing power. Efficiency is however conservatively assumed to be unchanged.

The effect of $p$ on the efficiency-power relationship for the constant-$h_A$ case is shown in Fig. 11. As expected, with finite $p$ the power is reduced from the case when the adiabatics take no time, with greater effect at low
efficiency, high power situation. However, even at $p = 4$, the difference is hardly noticeable whenever efficiency is greater than 80%.

Another key assumption made in this paper is that $h_A$ is a constant or only a function of gas volume. While the heat transfer area being volume dependent is accurate, the heat transfer coefficient is a function of other factors such as speed, density, temperature, viscosity and conductivity, etc. Some correlations for different porous media as heat exchangers can be found in [22], [10], [23]. To accommodate such general cases as well as to take into consideration the physical limitations in compression/expansion speeds, the optimal efficiency-power trade-off problem can be solved numerically either using generic nonlinear optimization algorithms (after parameterizing the trajectories) [16], [14]; or using dynamic programming [17]. Interestingly, even with complex heat transfer correlation and limits in compression/expansion rates, the optimal solutions also consist of maximum rates at the beginning and the end, and relatively slow rate in between. These are similar to the AIA or ApIA trajectories that are derived for the simplified case in this paper.

To implement the optimized trajectories using the liquid piston compressor/expander concept, only the displacement of liquid pump/motor needs to be adjusted in real-time to control flow rate. This operation is not energy intensive. One issue, however, is that optimal trajectories typically require large flow rates and hence larger variable displacement pump/motors. This drawback can be mitigated with a combined solid piston and liquid piston approach [24].

The benefits of applying optimized compression trajectories have been validated experimentally in [25], [26] for the low pressure (10bar) and the high pressure (200bar) settings respectively. Optimal trajectories were shown to double the power densities for the same efficiency, or to increase efficiency by 4-5% for the same power. These gains are consistent with the expectations based on the limitations in maximum flow rates and the heat transfer capabilities under the test conditions.

The results for the air volume dependent $h_A(V)$, $h_A' \geq 0$ case in Theorem 2 is a direct extension to the constant $h_A$ case in Theorem 1. However, for the generic case where $h_A'$ can be negative, the result is weaker, since the volume trajectories are restricted to be monotonic to ensure that ApIA is optimal. The restriction is needed because of the possibility that $(T - T_0) > 0$ and $(T - T_0) < 0$ can both be feasible solutions when $\partial h_A(V) / \partial V \neq 0$ and we have not ruled out that the optimal trajectories can involve switching between these two branches. Our conjecture
is that ApIA are indeed optimal even without the restriction that trajectory be montonic. This, however, has not been proved. In any case, it is expected that in practical situations, \( hA' \geq 0 \) is a reasonable assumption.

VII. CONCLUSIONS

In this paper, Pareto optimal trajectories for compressing or expanding gas that are Pareto optimal with respect to efficiency and power are obtained for the cases that the \( hA \), the product of heat transfer coefficient and heat transfer area, is a constant or only a function of volume. The optimal solutions consist of adiabatic steps sandwiching either an isothermal or a pseudo-isothermal step. Analytic solutions for these solutions are obtained. A case study motivated by compressed air energy storage application for wind turbine shows that the optimal solutions can increase power density 5 to 15 times over ad-hoc trajectories without sacrificing efficiency. These solutions can be extended for more complex heat transfer situation with numerical based solutions but the analytical solutions for these idealized cases offer important insights.

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