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Research Article

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DOI: https://doi.org/10.21203/rs.3.rs-820353/v1

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Energetics of water in the Solar System

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Water is vital for space exploration, from drinking to fuel reformation, and is naturally abundant in the Solar System¹–¹⁶. While in-situ resource utilization (ISRU) requires vastly less energy than transporting resources, the energetics has scarcely been explored besides on Earth and limited analysis on Mars’ vapor. Here, we develop a thermodynamic framework to quantify the energy requirements for resource extraction from 18 water sources on 11 planetary bodies. We find that desalinating saline liquid brines, where available, could be the most energetically favorable option and the energy required to access water vapor can be four to ten times higher than accessing ice deposits. While desalination energetics are highly sensitive to salt concentration, we show that desalination energetics only vary by a factor of 2 with respect to the type of salt present. Additionally, unlike chemical mixtures, the minimum energetics are insensitive to composition in physical mixtures (e.g., ice-regolith and inert vapor mixtures). Additionally, by deriving and computing the equation-of-state for pure water, we extend the least work estimates of atmospheric water harvesting by 94°C lower than previous studies that depend on predetermined databases. The presented approach and data may inform decisions regarding water harvesting, habitation, and resource reformation.

Keywords: In-situ resource utilization, space exploration, water, thermodynamics, least work
Stable sources of water in the Solar System can generally exist as saline liquid water brines, water vapor in the ambient air, or as water-ice. In many cases, liquid water sources solely exist deep underground and are combined with a variety of complex salts. Water vapor can be found in many atmospheres, but generally occurs in sparse quantities. Water-ice, on the other hand, is the most common form. It can be found in ice caps, craters, clouds, or small bodies in space. Space exploration and research has derived estimates of water temperature, pressure, and mixture composition on various bodies in the Solar System.

Prior literature has examined the water vapor properties including enthalpy, but this is limited in creating an understanding of the minimum energy requirements for extraction. On Earth, we have a robust understanding of the minimum energy requirements, but it is limited to air mixtures at Earth-standard temperatures and pressures. Understanding the properties of water in extreme environments, where it exists as highly saline mixtures, in high pressure environments (>100 MPa), and at high (>1000K) and low (<50K) temperatures, is still a primary research objective in astrophysics and physical chemistry. Overall, water in the Solar System is commonplace, yet thermodynamically complex, and the analysis of pure water extraction consequently varies significantly.

The least work framework is derived from the combination of the first and second laws of thermodynamics. It quantifies the exergy, or thermodynamic minimum energy, required to do a process and is computed using the properties of the water source that is used. Exergy-based analyses have been used in desalination and atmospheric water harvesting to compare the efficiencies of dissimilar processes but have not been used to evaluate the energetics of different water sources.

In Eq. 1, $W_{\text{least}}$ represents the minimum energy requirement, or least work, needed to obtain water from a given water source. $G$ is the Gibbs free energy, or embodied thermophysical energy, of water in a given environment or mixture. The Gibbs free energy is a function of the temperature, pressure, and chemical activity. The isothermal separation step is defined by the feed (input), permeate (pure water), and brine (reject). Subscript $f$ refers to the feed (f) or naturally occurring water-mixture. $p$ refers to the permeate, or pure water. $b$ refers to the brine (b) or reject – water-mixture after pure water is removed. The subscript Earth denotes the desired final state of liquid water at: Earth standard temperature (300K) and pressure (1 bar). $r$ signifies the fractional recovery of pure water from the bulk, feed mixture. $g_{\text{planet}}$ and $h$ respectively signify the acceleration due to gravity and relative height between the source and the surface of a given planetary body. The three grouped terms represent isothermal separation, heating of homogenous composition, and a change in gravitational potential.

In this work, we consider the least work of harvesting water from its existing state on a planetary body to the desired state at the given surface with Earth-standard temperature and pressure, as shown by Fig. 1. Extending this framework, we apply water mixture property models for extreme
conditions (low temperatures, high salinities, high pressures) to understand energy viability for water harvesting in extraterrestrial environments.

Fig. 1. Least work of water harvesting A. The two plots describe an upper and lower bound for the least work of desalination for liquid water mixtures of relevant two-component electrolyte solutions in the solar system. The lower and upper bounds are found by comparing the least work of ten binary aqueous solutions that are relevant to existing liquid water sources in the solar system. The axis bounds were limited to provide a meaningful comparison, since solubility varies for each species. B. The contour of least work is shown for water extraction from water vapor in a planet body’s atmosphere. The relative humidity represents the vapor pressure as a fraction of the saturation pressure at a given temperature. The axes maximize the range of validity of the thermodynamic models. The blue-green-yellow color contour (0–12 MJ/kg) numerically matches values in part A. C. Least work required to obtain water from pure ice is shown as a function of the ambient temperature. The desired temperature is assumed to be 300K (average temperature on Earth). Each subfigure considers the case where the water source is on the surface of the planet (in this, the change in gravitational potential is negligible).

The material phase of the source (solid, liquid, vapor) is the dominant factor for the energy requirements of pure water extraction, as described by Fig. 1. The energy requirement for
extracting pure water from concentrated liquid mixtures is generally one to two orders of magnitude lower than extracting from water-ice or water vapor. The energy requirement for extracting water from water vapor vastly ranges from near 0 (humid) to over 600 kJ/kg (arid).

As the temperature of the ambient environment approaches the desired temperature (assumed to be Earth standard 300K), the heating requirements decrease exponentially. Liquid source energy requirements are not as sensitive to temperature as they are to composition. This is due to the fact that water at Earth’s average temperature (300K) naturally exists as a liquid, and therefore have lower heating requirements (< 10 kJ/kg).

The molar concentration of a liquid water mixture is the primary factor in determining the energy requirement of extraction. The species of salt present has only a small impact, by less than a factor of two, as shown by the difference between the plots in Fig. 1A. This is explained by the variation in ion activity according to the Debye–Hückel theory and the Pitzer-Kim model. As a result, increasing the brine salinity, irrespective of which salt, proportionally increases the least work, within the range of conditions investigated. The separation energy for solutions increases non-linearly at high molalities, as shown by the increasing contour slope at high salinities. For most cases, the energy required to separate salts from liquid water mixtures is a larger proportion of the total energy requirement, especially for near Earth-standard conditions. This analysis does not account for the influence of organic materials which may be found in various bodies of water.

For water vapor, near-saturation conditions lead to the lowest separation energy requirements, with the least work approaching zero at saturation (RH = 100%). The separation energy requirement increases significantly below a relative humidity of approximately 20% and above 300K, as shown by Fig. 1B.

The absolute pressure of the water source and its environment mostly influence the phase-change regime (solid-liquid, solid-vapor, liquid-vapor). Changes in pressure within each regime have negligible effects in liquids and solids due to incompressibility. However, extreme pressures in liquid brines yield high solubility and ion activity, which may increase the least work. Ice is nearly incompressible, however extreme pressures (>100 MPa) may slightly decrease the required work.
Fig. 2: Comparison of least work on planetary bodies with known conditions. A The least work energy consumption, modeled by Equation 1 for each considered source, is plotted on a logarithmic scale, with the mean value shown. The averages for water-ice and water vapor sources are depicted in light blue and orange, respectively. Each colored bar is separated into up to three components (heating, separation, and gravitational energy), representing the energy contributions, to the total least work energy. When a source is not available on a given planet or an energy component of least work is zero, the respective color or bar is left out. Error bars represent a single standard deviation of energy requirements. Variation in dynamic weather conditions uses uniform distributions of parameters within observed ranges (Materials and Methods, Table S1 – S3). B The original sources of data are classified into categories based on the type of vehicle that was used.

The depth, or elevation, was considered for specific cases where the water source is not at the surface of the planetary body (Europa, Ganymede, Enceladus, etc.) or the elevation of the surface is unclear (Jupiter, Uranus). Gravitational potential energy is a significant factor in the energetics and is independent of the phase. As shown by Fig. 2, this energy requirement is most significant for Ganymede, where the thickness of the ice shell layer may be 800 km thick. The gravitational energy requirement varies significantly, up to two orders of magnitude. The acceleration due to gravity on the moons with liquid water is approximately $0.1 \text{–} 1.5 \frac{m}{s^2}$, while the gravitational acceleration on Uranus and Jupiter are approximately $9 \text{ and } 25 \frac{m}{s^2}$, respectively. The location of the water source, relative to the surface, is unique to each planet. For example, the thickness of an ice layer (10-800km), depth of a brine deposit, or altitude of a cloud layer are influenced by a number of factors including the dynamics of planetary formation, internal heat fluxes, and weather. We note that in niche circumstances, a theoretically ideal system may be able to bypass gravitational pumping requirements. This would include transporting liquid from the bottom of an ocean or vapor through an atmosphere, assisted by a natural pressure gradient.
Since the modeled desired state is set to average Earth conditions (300K, 1 bar), the most energetically viable source of water is liquid water on Earth, as shown by Fig. 2A. Similarly, on planetary bodies where liquid sources are available, liquid water is usually the most viable. These bodies include Mars (as sparse subsurface brines) and the moons of Jupiter and Saturn (as subsurface oceans). Ganymede is the exception due to its thick ice shell (800 km) posing a large contribution to the gravitational energy requirement. Other rocky bodies – the Moon, and Mercury – are limited in what may be extracted, since water-ice is the primary form that is available. Furthermore, Venus is fundamentally the least favorable, as water vapor is the only water option. However, acquiring such water may still be desirable, as the least work of such intensive vapor extraction is still significantly less than the energy required for deep space transport by rockets.

A lower bound for the theoretical minimum energy to take an object into space is the kinetic energy associated with escape velocity. On Earth, this is 11.19 km/s or approximately 62,600 kJ/kg payload. Modern chemical rockets require significant amounts of additional fuel mass, which effectively increases the energy per payload mass. In contrast, the energy required per mass of water carried by a deep space rocket may be anywhere from 100 to over 10,000 times greater than in situ resource utilization from the water sources investigated in this work.

The least work analysis here uncovers trends in the thermodynamics of water extraction. It describes the theoretically ideal physics, agnostic of any specific technology. The framework considers the energy change of the sample of water itself. The abundance of available thermodynamic work in the solar system, such as sunlight, may be harnessed to satisfy the energy budget. Realizable engineering systems will include both process and path specific requirements on top of the thermodynamic minimum. Examples of such practical inefficiencies include frictional and heat losses and limitations of energy reuse. The implementation of such extraterrestrial systems may be faced with “astronomical” infrastructure challenges. Accessing sources of water at great depths and filtering complex salts at high salinities will pose continued issues. Additional study is needed to understand the infrastructure requirements to establish Earth-like conditions on the surface of another planet. When current limitations are surpassed, the ability to access water on other worlds will unlock a vast range of possibilities for the exploration of our Solar System.

While the presented results discuss a widely applicable range of conditions observed on Earth and other planets, more states of liquid water exist and are yet to be thoroughly characterized. Specifically, at extremely high (>10,000 K) and low (<50K) temperatures and high pressures (>100 MPa), characterizing the free energy of water treads into unknown territory. Supercooled liquid states and salt-glass are relevant to many cold planets and are created by path-specific cooling that has further complexities.

The least work framework, for the minimum energy to obtain pure water, helps prioritize water sources by their macro properties. The parametric study of energetics (Fig. 1) and discrete case studies (Fig. 2) provide a new perspective for prioritizing the exploration of known and theoretical worlds. This work serves as a basis for modeling resource harvesting in harsh and unknown environments. Further investigation should help more clearly quantify degrees of habitability for humans based on the energy requirement of obtaining water. The input parameters for the models
presented in this paper can be verified with a more in-depth characterization of the given sources of water. The exploration of the engineering constraints of systems can provide a means for quantifying tradeoffs between the accessibility and energetics of water extraction. This understanding will help to drive the future decisions concerning water harvesting and resource (oxygen and fuel) reformation.

**Methods**

To analyze the energetics of water extraction in the Solar System, we mapped the least work with respect to input conditions are common to water sources in the Solar System. Using the macro properties of various water sources, we conducted a case study to compare the energetics of water harvesting from each source. Data was obtained from various space exploration initiatives (referenced in main text). Models referenced established thermochemistry databases with Engineering Equation Solver (EES) and PHREEQC. Property models were additionally validated with CoolProp and EES, which are ASHRAE and NIST validated thermal fluid property databases. To quantify uncertainty, we used a Latin hypercube approach to sample evenly across the range of conditions. This method is commonly used to quantify uncertainty in higher dimensions with a limited number of samples.

**Model Derivation**

For each existing body of water of known pressure, temperature and composition, a black box is used to represent input (i.e. feed) and output streams, (i.e. brine and permeate) with the corresponding energy input. By solving the first and second laws of thermodynamics for a both internally and externally reversible system, the minimum energy for obtaining drinkable water simplifies to a change in Gibbs free energy between the input and output states plus any change in gravitational potential. This calculation assumes the final destination of the water is at the world’s surface. For systems without a clearly defined surface or extremely high surface pressures, such as the gas giants, ice giants, and Venus, the final destination occurs at an elevation associated with 1 bar of pressure. The initial elevation is taken to be the approximated location of the water source, via measurement or models.

\[
G(T, P, C) = H(T, P) - T_0 S(T, P) + \sum_i C_i \mu_i
\]  

Where \( G \), the Gibbs free energy is defined as a function of the thermodynamic state. \( H \) represents the enthalpy of the defined state, the subscript \( o \) represents the dead state temperature, or ambient temperature, \( S \) represents the entropy at the defined state, \( \mu_i \) represents the chemical potential, \( T \) is the solution temperature, \( P \) is the solution pressure, and \( C \) is the fractional composition of each constituent. The least work is defined as a balance of Gibbs free energy.

\[
W_{\text{least}} = W_{\text{sep}} + W_{\text{heat}} + W_{\text{grav}}
\]

The least work is divided into separation, heating, and gravitational components.
\[
W_{\text{sep}} = \lim_{r \to 0} G_p(T_0, P_0, 0) - \frac{1}{r} G_f(T_0, P_0, C_0) + \frac{1-r}{r} G_b(T_0, P_0, C_0^*), \tag{3}
\]

\[
W_{\text{heat}} = G_{\text{Earth}}(300K, 100 \text{ kPa}, 0M) - G_p(T_0, P_0, 0) \tag{4}
\]

\[
W_{\text{grav}} = \int m g dx \tag{5}
\]

The subscripts: \(\text{sep}, \text{heat}, \text{and grav}\), represent thermodynamic work, heating, and gravitational potential energy. Where \(r\) is the fraction of ambient water that is converted to pure water and \(C_0^*\) is calculated based on \(C_0\) and \(r\). \(g\) and \(x\) signify the acceleration due to gravity and relative position of a water source to the surface. The subscripts

For desalination, or water sources that are chemically combined with salts, the separation component of least work can be expanded with the Pitzer formulation of Gibbs free energy. \(^\text{23}\)

\[
w_{\text{sep}} = \frac{1-r}{r} \frac{RT_0}{1 + \sum b_i M_i} \left( \Sigma b_i \ln a_i + \frac{1}{M_w} \ln a_w \right)_b - \frac{1}{r} \frac{RT_0}{1 + \sum b_i M_i} \left( \Sigma b_i \ln a_i + \frac{1}{M_w} \ln a_w \right)_f \tag{6}
\]

The activities of a species and its molality are represented by \(a\) and \(b\). Solutes are denoted by the subscript \(i\), while water on a per mass basis is denoted by \(w\). The solute concentrations, solute activities and solvent activity of the brine depend on the recovery ratio \((r_i)\) of the separation process. \(R_i, T_0,\) and \(M_i\) denote the universal gas constant, temperature of the source. Separation work values are evaluated at small recovery ratios \((r = 0.075, 0.05, 0.025)\) and extrapolated to zero to obtain the minimum least work at infinitesimal recovery. \(^\text{22}\)

Similar to desalination, vapor extraction processes utilize three streams of fluid in analysis. The input is the system’s atmosphere, and the outputs are pure water and dehumidified atmosphere. To evaluate this mathematically, the work component of the process is evaluated as a change in Gibbs free energy of system, as shown below.

\[
W_{\text{sep}} = \lim_{r \to 0} G_p - \frac{1}{r} G_f + \frac{1-r}{r} G_b \tag{7}
\]

Water-ice on other worlds is assumed to be high purity surface ice deposits. Unique cases of ice-soil mixtures require thorough chemical characterization of the soil and solution properties. Since no separation is needed, the recovery ratio does not affect the energetics and therefore is implemented with \(r = 1\) for simplicity.

**Property models**

Property relationships for liquid water are extracted from PHREEQC with the FREZCHEM database for electrolyte solutions. Property relationships for ice and vapor are derived analytically from Maxwell’s equations. \(^\text{12, 19, 32}\).
For water vapor, the standard form of a real gas with a compressibility factor \((Z)\) is used. The 2-term virial form is used and described in Eq 14, 15.

\[
\frac{Pv}{RT} = Z
\]  

Where \(Z\) is the compressibility factor, which represents deviation from ideal gas behavior. \(v\) is the specific volume and \(R\) being the gas constant for water vapor. This equation is rearranged for volume and the partial derivative with respect to temperature is taken, while holding pressure constant.

\[
\frac{\partial v}{\partial T} \bigg|_P = \frac{ZR}{P}
\]

The differential forms for changes in entropy and enthalpy are simplified with the compressibility factor, below.

\[
ds = \frac{c_p}{T}dT - \frac{\partial v}{\partial T} \bigg|_P dP = \frac{c_p}{T}dT - \frac{ZR}{P}dP
\]

\[
dh = Tds - vdP = c_pdT
\]

Combining these equations yields a differential form of Gibbs free energy, with respect to a dead state \(T_0\). In this section, lower case \(g\) represents the specific Gibbs free energy on a mass basis.

\[
dg = dh - T_0ds = c_pdT - c_pT_0 \frac{dT}{T} + ZRT_0 \frac{dP}{P}
\]

Integrating this differential form from an arbitrary dead state to the ambient temperature yields the following form of free energy. This implicitly assumes that the specific heat capacity function is constant, linear, or symmetric over the considered temperature range.

\[
\Delta g = g - g_0 = c_p \left( \Delta T - T_0 \ln \frac{T}{T_0} \right) + ZRT_0 \ln \frac{P}{P_0}
\]

Where the subscript 0 represents an arbitrary dead state and \(\Delta\) refers to the difference between the state and the dead state. For vapors, the compressibility factor is modeled by a 1st degree Taylor series expansion about the pressure \(^37\).

\[
B' = \left[ 0.44687 - \left( \frac{565.965}{T^2} \right) \times 10^{\frac{10800}{34900+7^2}} \right] \times 10^{-5}
\]

Where \(B'\) is the virial coefficient as a function of temperature, expressed in \(\text{Pa}^{-1}\). This correlation was used by Wexler (1977) to predict the compressibility factor within 0.01% over a wide range of temperatures (173K – 600K) \(^37\).
The vapor pressure of ambient water is used as the dead state pressure. This is found via the Buck correlations for saturated water vapor over liquid water or ice \(^{38}\).

To model the free energy of water ice, the sample is assumed to be incompressible, which simplifies the Gibbs equation to only a function of temperature. The associated specific heat for ice is used, instead.

\[
\Delta g = g - g_0 = c_p \left( \Delta T - T_0 \ln \frac{T}{T_0} \right)
\]  

(16)

**Error analysis**

The variable conditions of each planet are considered with a sensitivity analysis. A Latin hypercube sampling method was used to reduce the number of calculations needed to capture high dimensional uncertainty. The built-in MATLAB Latin hypercube tool, *lhsdesign*, was used to choose the sample conditions based on a given range. Using the range, the tool splits the high dimensional space into a \(n \times n\) grid and samples a random point such that each row and column is equally distributed. The model computes the least work as a function of the chosen input source conditions. Then, the mean and sample standard deviation are computed for each source. The ranges of model input conditions are listed in Table S1. The ranges of conditions for each planet are considered to be static and uniform, rather than either spatially or temporally weighted. Therefore, the described uncertainty analysis has uniform probability and error in this case represents a range of possible values rather than a statistical interpretation.

The equation of state formulation for vapors is validated against the CoolProp property database. CoolProp contains water vapor and air properties and is thoroughly validated against ASHRAE standards. The activity values from PHREEQC are compared across various database files and the least work for saline brines are similarly compared with Mistry, Hunter, Lienhard (2013) \(^{23}\). Visualization of property modeling errors are described in Fig. S2 - S6.

**Model limitations**

Limitations in the models are largely associated with estimates in thermodynamic properties of water. To generalize to planets with unknown atmospheres, we assumed water is inert in the vapor mixture and used partial properties to simplify property models. Validating this assumption, we find that water vapor generally exists in low temperature or low humidity environments. At low vapor pressures and temperatures, such as those considered in this work, water vapor behaves nearly like an ideal gas. For real mixtures with highly volatile gases, the interspecies bonding energy will lead likely to a slightly higher least work prediction in saturated and high temperature environments. Fig. 1C is most accurate at lower temperature and humidity. The error may be near 5\% at low concentrations (RH < 40\%), as shown by a comparative study with real air mixtures (Fig. S7). Additionally, to generalize property models in liquid brine mixtures, we considered binary salt mixtures at varying salinities in Fig. 1A. To understand extraction energy requirements for more complex, tertiary, and quaternary salt mixtures, the specific composition of the mixture is required. Further experimental study is needed for accurate predictions of the thermodynamic properties of such mixtures. Finally, the property models for water-ice consider ice in its pure form. This is a reasonable assumption in many cases, like the icy moons of Saturn and Jupiter. The
thermodynamic state is also limited in that it cannot capture the energetics of physically mixed
substances like regolith-water-ice. For liquid and ice sources that naturally exist in clathrates or
other physically absorbent structures, such as regolith, zeolites, or metal organic frameworks, the
structure-specific adsorption energy barrier is an additional consideration

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Acknowledgments: The authors thank Dr. David Catling and Dr. Jonathon Toner for permission to use their suite of models on the chemistry of brines and high salinity sources on other planets. The authors also thank James Zampa, Sophia Gripp, Anirwin Yekkala, and Jiyoon Im for assistance in data analysis, acquisition, and visualization. Additionally, the authors thank Dr. Alison Bramson, Dr. Felice Frankel, and Dr. Michael McDonald, Xavier Morgan-Lange, and Debraliz Isaac-Aragones for feedback through the drafting process. The authors acknowledge Purdue University EVPRP and the Purdue University Mechanical Engineering.

Author contributions: Akshay K. Rao: Methodology, Software, Validation, Formal Analysis, Investigation, Writing, Visualization, Project Administration. Abhimanyu Das: Methodology, Software, Validation, Investigation, Writing. Owen R Li: Validation, Investigation, Writing, Visualization. David M. Warsinger: Conceptualization, Methodology, Resources, Writing, Supervision, Funding Acquisition.

Competing interests: The authors declare no competing interests.
Data and materials availability: Code and data can be found within the supplementary materials or on GitHub upon publication: https://github.com/Warsingerlab/. The authors will clarify any additional information upon request.

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