Zero-Emission Gasoline-Powered Automobiles

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Abstract. With the future advent of atomically precise manufacturing (APM) using nanofactories, gasoline-powered automobiles with conventional internal combustion engines could be manufactured or retrofitted with nanomachinery that converts the cars into zero-emission vehicles. An array of nanoscale molecular pumps called sorting rotors would extract all carbon dioxide and other noxious combustion byproducts (e.g., CO, NO_x, and unburned hydrocarbons) from the post-catalytic-converter engine exhaust stream during vehicle operation and compress these gases into an onboard pressure vessel at 1000 atm. An onboard ~0.03 m^3 sorting rotor filtration system and the ~0.20 m^3 onboard pressure vessel draw ~9.3 kW of power from a 200 horsepower vehicle when operated continuously in typical highway or city driving, using only 21% of the chemical energy stored in 16 gallons of gasoline to achieve zero net emissions. The compressed gases are later disgorged at a service station when the automobile stops to refuel. The service station locally synthesizes gasoline from the compressed exhaust gases, also on a zero-emissions basis, to refuel the cars. Service stations each need ~10 MW to support local gasoline recycling, requiring an additional ~1 TW of electrical capacity to be added to the U.S. national power grid, an 81% increase from 2024 levels, assuming 100,000 service stations servicing 200 million cars that each refuel once every 10 days.

Cite as: Robert A. Freitas Jr., “Zero-Emission Gasoline-Powered Automobiles,” IMM Report No. 57, 8 Apr 2025; http://www.imm.org/Reports/rep057.pdf.

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1. Introduction

Gasoline powered automobiles consume hydrocarbon fuels and release carbon dioxide and other noxious exhaust emissions into the atmosphere, creating air pollution and potentially contributing to global warming.[1] One often-proposed solution is to switch to battery-powered electric cars, which themselves have zero emissions[2] and may provide transportation at comparable or cheaper operating costs per distance traveled.[3] But as a store of energy, gasoline offers nearly 50 times higher energy density than batteries.[4]

This suggests an interesting possibility: We could use atomically precise manufacturing[5] (APM), once it becomes available, to build or retrofit gasoline-powered automobiles with specialized nanomachinery equipment that converts these cars to zero net emissions when operated, including offboard synthesis of gasoline as a carbon-neutral fuel[6] from the emissions. The present document describes how this might work.

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[1] https://en.wikipedia.org/wiki/Causes_of_climate_change#Carbon_dioxide.
[2] https://en.wikipedia.org/wiki/Zero_emission.
[3] https://www.nrdc.org/stories/electric-vs-gas-cars-it-cheaper-drive-ev.

[4] Tesla's Model Y electric car has an 82 kWh battery with a volume of ~0.4 m^3, giving an energy density of **0.74 MJ/L**, far lower than the ~**35 MJ/L** energy density of gasoline.

[5] Drexler KE. Nanosystems: Molecular Machinery, Manufacturing, and Computation, John Wiley & Sons, New York, 1992; Chapter 14, "Molecular Manufacturing Systems"; https://www.amazon.com/dp/0471575186/. Freitas RA Jr., Merkle RC. Kinematic Self-Replicating Machines. Landes Bioscience, Georgetown, TX, 2004, Section 5.7 "Massively Parallel Molecular Manufacturing"; http://www.MolecularAssembler.com/KSRM/5.7.htm. Freitas RA Jr., Merkle RC. A minimal toolset for positional diamond mechanosynthesis. J Comput Theor Nanosci. 2008;5:760-861; http://www.molecularassembler.com/Papers/MinToolset.pdf. Freitas RA Jr. Cryostasis Revival: The Recovery of Cryonics Patients through Nanomedicine. Alcor Life Extension Foundation, Scottsdale AZ, 2022; Section 1.3.2, "Nanofactories"; https://www.alcor.org/cryostasis-revival/. Freitas RA Jr., Merkle RC. Nanofactory Collaboration website; https://www.molecularassembler.com/Nanofactory/index.htm.

[6] https://en.wikipedia.org/wiki/Carbon-neutral_fuel.

2. Exhaust Products of Gasoline-Powered Automobiles

Consider an "average" U.S. passenger car equipped with a 200 horsepower engine[7] (P_{engine} = 149.1 kW) and a V_{tank} = 16 gallon (0.0606 m^3) gas tank[8] filled with $M_{gasoline} = \rho_{gasoline} V_{tank} \sim 44.2$ kg of gasoline of density $\rho_{gasoline} \sim 730$ kg/m^3 at 15 °C,[9] that will liberate $E_{gasoline} = M_{gasoline} E_{D,gasoline} \sim 2120$ MJ of energy when combusted in ambient air, taking the specific energy of gasoline as $E_{D,gasoline} \sim 47.895$ MJ/kg.[10]

Modern gasoline engines have a maximum thermal efficiency of more than 50%, but most road legal cars only achieve $\varepsilon_{car} \sim 25\%$ (range 20-40%) efficiency, with ~70% of total power emitted as heat without being turned into useful work such as turning the crankshaft.[11] Typical highway or city driving may employ only a small fraction of the engine's maximum power, e.g., 20-40 horsepower to cruise at 65-75 mph. If we assume a power level of ~30 horsepower ($P_{car} \sim 22.4$ kW), then the car can be driven for $t_{drive} = \varepsilon_{car} E_{gasoline} / P_{car} \sim 23{,}700$ sec = 6.6 hr of continuous operation in typical highway or city driving on a single tankful of gasoline.

The combustion of gasoline in air can be closely approximated as the complete combustion of octane in oxygen, as:

$$\begin{gathered}
2\ C_8H_{18}\ \text{(octane)} + 25\ O_2 \rightarrow 16\ CO_2 + 18\ H_2O + E_{gasoline} \\
2\ (0.114\ \text{kg/mole}) + 25\ (0.032\text{kg/mole}) \rightarrow 16\ (0.044\ \text{kg/mole}) + 18\ (0.018\ \text{kg/mole}) \\
0.228\ \text{kg}\ C_8H_{18} + 0.8\ \text{kg}\ O_2 \rightarrow 0.704\ \text{kg}\ CO_2 + 0.324\ \text{kg}\ H_2O \\
44.2\ \text{kg}\ C_8H_{18}\ \text{[tank]} + 155.1\ \text{kg}\ O_2 \rightarrow 136.5\ \text{kg}\ CO_2 + 62.8\ \text{kg}\ H_2O
\end{gathered}$$

The total mass of air inhaled by the car during the combustion of one tank of gasoline is $M_{air} = M_{O2} / f_{O2} \sim 672.0$ kg, taking $M_{O2} \sim 155.1$ kg with the oxygen content of dry air expressed as a mass fraction as $f_{O2} \sim 0.2314$,[12] and assuming ~0.25% by mass ($M_{H2Oatm} \sim 1.7$ kg) of atmospheric water in typical non-dry air.[13] Trace amounts of carbon monoxide (CO), nitrogen

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[7] Smith G. The Average Horsepower in American Cars IS Higher Than You Think. CarBuzz, 2024 Aug 11; https://carbuzz.com/the-average-horsepower-in-american-cars-is-higher-than-you-think/.

[8] https://en.wikipedia.org/wiki/Fuel_tank#Passenger_vehicles.

[9] Volume correction factors – gasoline. Innovation, Science and Economic Development Canada, Measurement Canada, July 2018; https://www.ic.gc.ca/eic/site/mc-mc.nsf/425f69a205e4a9f48525742e00703d75/5ea3aeed72375148852582d00055d6a4/$FILE/VCF_Gasoline_Ethanol-Blends.pdf.

[10] Freitas RA Jr. Energy Density. IMM Report No. 50, 25 June 2019; Section 4.2.3 Ambient Chemical Combustion, Table 29; http://www.imm.org/Reports/rep050.pdf.

[11] https://en.wikipedia.org/wiki/Engine_efficiency#Gasoline_(petrol)_engines.
[12] https://en.wikipedia.org/wiki/Atmosphere_of_Earth#Composition.
[13] https://en.wikipedia.org/wiki/Atmosphere_of_Earth#Composition.

oxides (NO_x), and unburned hydrocarbons (UHC) are usually present in tailpipe exhaust gases,[14] though these can be less than 1% by mass during complete combustion. Assuming typical emissions for gasoline engines operating under real-world conditions, the mass of tailpipe emissions ($M_{tailpipe}$) from one tankful of gasoline might include (1) $M_{CO} = f_{CO}\ M_{OxCombProds} \sim 4$ kg CO, taking f_{CO} = 1-3% by mass in the exhaust gases, (2) $M_{NOx} = f_{NOx}\ M_{OxCombProds} \sim 0.4$ kg NO_x, taking f_{NOx} = 0.1-0.3% by mass in the exhaust gases (typically 90-95% or ~0.37 kg as NO, 5-10% or ~0.03 kg as NO_2, and <1% as N_2O and other oxides which we will ignore here), and (3) <0.25% of unburned hydrocarbons, or $M_{UHC} \sim 0.5$ kg of UHC,[15] where total oxidized combustion products are $M_{OxCombProds} = M_{CO2} + M_{H2O} + M_{CO} + M_{NOx} + M_{UHC} = 204.2$ kg, with $M_{CO2} \sim 136.5$ kg CO_2 and $M_{H2O} \sim 62.8$ kg H_2O.[16] Sulfur compounds and other trace elements will not be present in the exhaust if the "gasoline" is chemically pure octane, as assumed in this example. The total tailpipe emission is then $M_{tailpipe} = M_{air} - M_{O2} + M_{OxCombProds} = 721.1$ kg. The tailpipe emissions also include unreacted components totaling $M_{unreactedair} = M_{N2} + M_{Ar} + M_{CO2atm} + M_{H2Oatm} = 516.9$ kg, where $M_{N2} = 506.2$ kg (nitrogen) and $M_{Ar} \sim 8.6$ kg (argon), and a mass fraction of 626 ppm[17] of atmospheric CO_2 (M_{CO2atm} = (636 ppm) (M_{air}) ~ 0.4 kg) in the inhaled air gets passed through unreacted, as summarized in Table 1.

Table 1. Approximate mass and molecular weight (MW) of the entire exhaust stream from the complete combustion of one 16-gallon tank of gasoline in air.

Mixed Exhaust Component	**Mass (kg)**	**MW (kg/mole)**	**Mixed Exhaust Component**	**Mass (kg)**	**MW (kg/mole)**
Combustion CO_2	136.5	0.044	Atmospheric N_2	506.2	0.028
Combustion H_2O	62.8	0.018	Atmospheric Ar	8.6	0.040
Combustion CO	4.0	0.028	Atmospheric H_2O	1.7	0.018
Combustion NO_x	0.4	0.030	Atmospheric CO_2	0.4	0.044
Combustion UHC[18]	0.5	0.048	***Total*** ($M_{tailpipe}$)	***721.1***	*0.030*

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[14] https://en.wikipedia.org/wiki/Exhaust_gas.

[15] e.g., Sassykova LR *et al.* The main components of vehicle exhaust gases and their effective catalytic neutralization. Oriental J Chem. 2019;35(1); https://www.orientjchem.org/vol35no1/the-main-components-of-vehicle-exhaust-gases-and-their-effective-catalytic-neutralization/.

[16] The mass values given for CO, NO_x, and UHC are pre-catalytic converter amounts, providing a conservative design. A modern catalytic converter would eliminate most of these. This sizes the system for worst-case or real-world conditions where converters underperform.

[17] https://en.wikipedia.org/wiki/Atmosphere_of_Earth#Composition.

[18] Typical components of unburned hydrocarbons in combustion gases might include ~20% ethylene (C_2H_4), ~15% methane (CH_4), ~10% propylene (C_3H_6), ~5% benzene (C_6H_6), ~5% 1,3-butadiene (C_4H_6), ~3% toluene (C_7H_8), ~3% acetylene (C_2H_2), ~2% formaldehyde (CH_2O), ~17% higher alkanes (avg C_6H_{14}), and ~20% other trace compounds; average molecular weight ~0.048 kg/mole with formula $C_{3.325}H_{6.6}O_{0.025}$.

To convert the car into a zero-exhaust vehicle, we insert between the catalytic converter and the tailpipe a filtration device containing a set of molecular pumps that would selectively remove M_{CO2} ~ 136.5 kg of combustion CO_2 gas from the exhaust stream, thus reducing the total CO_2 content of the exhaust stream by x_{CO2} ~ 99.7% from $M_{CO2} + M_{CO2atm}$ ~ 136.9 kg CO_2 down to M_{CO2atm} ~ 0.4 kg CO_2 (ambient level),[19] thus achieving zero net emission of CO_2 relative to normal atmospheric levels, by extracting $M_{CO2filter} = x_{CO2}\ (M_{CO2} + M_{CO2atm})$ ~ 136.5 kg of CO_2 from the exhaust stream. A second set of molecular pumps will also selectively extract most of the $M_{other} = M_{CO} + M_{NOx} + M_{UHC}$ ~ 4.9 kg of combustion CO, NO_x, and UHC gases from the exhaust stream. We'll assume that a removal rate of x_{other} ~ x_{CO2} = 99.7% constitutes effective "net zero" operation, since regulatory-approved EPA-mandated catalytic converters typically achieve only 90% removal of these gases in typical on-road performance.[20] This second set of molecular pumps will be removing $M_{otherfilter} = x_{other}\ M_{other}$ ~ 4.89 kg of CO, NO_x, and UHC gases, leaving only ~0.01 kg in the exhaust stream. In this scenario, $M_{compress} = M_{CO2filter} + M_{otherfilter}$ ~ 141.4 kg of harmful extracted exhaust gases are compressed into an onboard pressure vessel at 1000 atm pressure, and the remaining $M_{finalexhaust} = M_{tailpipe} - M_{compress}$ ~ 579.7 kg of exhaust gases (Table 2) are released into the atmosphere through the tailpipe. An amount of water necessary to satisfy the objective of zero net H_2O emissions for the vehicle is later extracted from the atmosphere at a distant service station, where the original gasoline fuel is mechanosynthetically reconstituted using compressed CO_2 that is transferred to the station from the car's onboard pressure vessel (Section 6).

Table 2. Approximate mass and molecular weight (MW) of remnant exhaust gases that are released into the atmosphere.

Mixed Exhaust Component	**Mass (kg)**	**MW (kg/mole)**	**Mixed Exhaust Component**	**Mass (kg)**	**MW (kg/mole)**
Combustion CO_2	0.0	0.044	Atmospheric N_2	506.2	0.028
Combustion H_2O	62.8	0.018	Atmospheric Ar	8.6	0.040
Combustion CO	0.008	0.028	Atmospheric H_2O	1.7	0.018
Combustion NO_x	0.0008	0.030	Atmospheric CO_2	0.4	0.044
Combustion UHC	0.001	0.048	***Total*** ($M_{finalexhaust}$)	***579.7***	*0.027*

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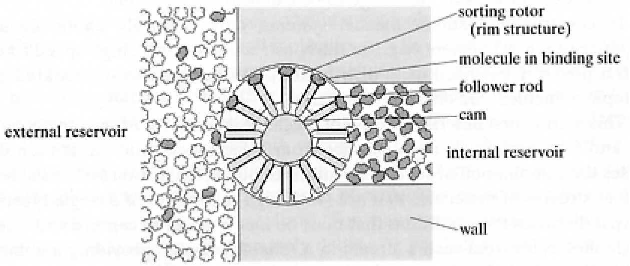
[19] $x_{CO2} = (M_{CO2}) / (M_{CO2} + M_{CO2atm})$ = (136.5 kg) / (136.5 kg + 0.4 kg) ~ 99.7%.

[20] Heywood JB. Internal Combustion Engine Fundamentals. McGraw-Hill, Second Edition, 2018; https://www.amazon.com/Internal-Combustion-Engine-Fundamentals-2E/dp/1260116107/.

3. Sorting Rotors for CO_2



Carbon dioxide molecules can be selectively removed from the exhaust stream using molecular pumps called sorting rotors,[21] classically illustrated (image, right) as a disk about 10 nm in diameter and about 3 nm thick having 12 binding site "pockets" along the rim that are exposed alternately to the source fluid at left and the receiving chamber at right by the clockwise axial rotation of the disk. Each pocket selectively binds a specific molecule when exposed to the source fluid at left. The rotor turns clockwise, moving the pocket containing the bound molecule through the wall from left to right. Once the binding site has rotated far enough to expose it to the receiving chamber at right, the bound molecules are forcibly ejected by rods (e.g., polyynes) thrust outward by the cam surface. Molecular sorting rotors can be designed from about 10^5 atoms (including housing and pro rata share of the drive system), measuring roughly 7 nm x 14 nm x 14 nm in size (volume $V_{rot} \sim 1372\ nm^3$) with a mass of $M_{rot} = 2 \times 10^{-21}$ kg.

Rotors turn at ~86,000 rev/sec with a conservative rim speed of 2.7 mm/sec and an almost negligible drag power of $\sim 10^{-16}$ watts against the fluid, sorting small molecules at a rate of $r_{sort} \sim 10^6$ molecules/rotor-sec with laminar flow, assuming 99% occupancy[22] of the binding sites at this rotor speed. Removing 99.7% of the CO_2 molecules from the exhaust stream requires up to $\Delta G = k_B T \ln(c_2/c_1) = 4.60 \times 10^{-20}$ J/molecule, taking $c_1 \sim 0.003$ atm, $c_2 \sim 1$ atm (normal engine exhaust pressure), T ~ 573 K (300 °C),[23] and $k_B = 1.381 \times 10^{-23}$ J/K (Boltzmann constant), so each rotor requires $P_{rot} = r_{sort}\ \Delta G \sim 0.046$ pW to operate continuously.

We must extract $n_{CO2} = M_{CO2filter}\ N_A\ /\ MW_{CO2} = 1.87 \times 10^{27}$ molecules of CO_2 and $n_{other} = M_{otherfilter}\ N_A\ /\ MW_{other} = 9.84 \times 10^{25}$ molecules of CO, NO_x, and UHC gases from the exhaust stream, taking $MW_{CO2} = 0.044$ kg/mole, $MW_{other} = 0.030$ kg/mole, and $N_A = 6.023 \times 10^{23}$ molecules/mole. This requires a maximum of $N_{rotors} = (n_{CO2} + n_{other})\ /\ r_{sort}\ t_{drive} = 8.30 \times 10^{16}$ sorting rotors of total mass $M_{rotors} \sim M_{rot}\ N_{rotors} = 0.166$ gm, total volume $V_{rotors} \sim V_{rot}\ N_{rotors} =$

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[21] Drexler KE. Nanosystems: Molecular Machinery, Manufacturing, and Computation. John Wiley & Sons, New York, 1992, Section 13.2, "Sorting and Ordering Molecules"; https://www.amazon.com/dp/0471575186/. Freitas RA Jr. Nanomedicine, Volume I: Basic Capabilities. Landes Bioscience, Georgetown, TX, 1999, Section 3.4.2, "Sorting Rotors"; http://www.nanomedicine.com/NMI/3.4.2.htm.

[22] If subsequent detailed analysis concludes that 99% binding site occupancy cannot be assured for all gas components at the specified rotor speed and exhaust gas concentration, the component gas partial pressures can be increased at least 1000-fold by pre-compressing the exhaust stream up to 1000 atm at a fairly modest energy cost (**Section 5**).

[23] Automobile exhaust gases are typically 300 °C to 600 °C as they exit the catalytic converter and 150 °C to 300 °C as they enter the tailpipe; e.g., https://www.jdpower.com/cars/shopping-guides/how-hot-does-a-car-exhaust-pipe-get.

0.114 cm^3,[24] and maximum power consumption $P_{rotors} = P_{rot} N_{rotors}$ = **3.8 kW** if the car is operated continuously in typical highway or city driving.

Even the most basic scaling analysis of the sorting rotor filtration system configuration gives reasonable flow rates. For example, the gas-facing interfaces of an array of 8.26×10^{16} sorting rotors can be packed onto square filtration membranes of total surface area $A_{array} = A_{rotor} N_{rotors}$ = 8.1 m^2, taking A_{rotor} = 98 nm^2 (= 7 nm x 14 nm), over which the exhaust gases may flow as the N_2 and H_2O molecules are 99% extracted from the exhaust gases by the array and ejected into the tailpipe. The square filtration membranes, each of surface area $A_{membrane}$ = 0.1 m^2, could be stacked inside a plenum containing with $N_{membrane} = A_{array} / A_{membrane}$ = 81 parallel membranes filling a cubical box measuring $L_{plenum} = A_{membrane}^{1/2}$ = 0.316 m on a side with volume L_{plenum}^3 = 0.0316 m^3 (~1.1 ft^3). Adjacent membranes inside the box would be separated by $d_{membrane} = L_{plenum} / N_{membrane}$ = 3.9 mm, leaving plenty of space for the 0.014 μm thick sorting rotors and additional nanomechanical infrastructure for delivering power and control beneath the filtration membrane surface. Exhaust gases will pass through the plenum at a velocity $v_{gases} \sim M_{tailpipe} / \rho_{gases} t_{drive} d_{membrane} L_{plenum} N_{membrane}$ ~ 49.5 cm/sec with a plenum transit time of L_{plenum} / v_{gases} = 0.639 sec, taking exhaust gas density ρ_{gases} ~ 0.616 kg/m^3 at 573 K (300 °C).

In conclusion, given advanced nanoscale machinery, we can physically separate CO_2 from exhaust in real-time.

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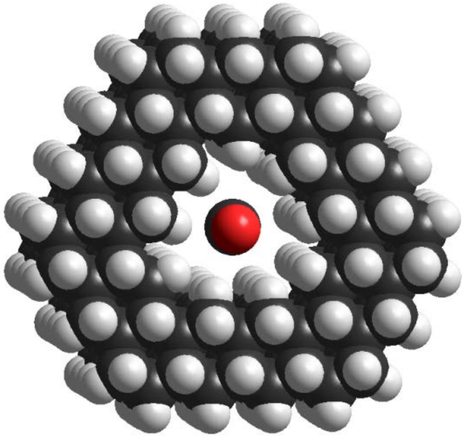
[24] While the rotors themselves occupy only ~10^{-7} m^3, practical packaging and the flow apparatus (see the following paragraph, above) raise the filter unit or cubic "plenum" volume to L_{plenum}^3 = 0.0316 m^3 (~1.1 ft^3).

4. Binding Site Design for CO_2

The strength of the binding of the target molecule to the artificial receptor site can be designed to be sufficient to achieve high occupancy of all pockets (e.g., 99%) at the given relatively low speeds of rotor rotation. The mechanical energy consumed to force the target molecule out of its binding site into the receiving chamber is delivered from the cam to the rods, but this energy is largely returned with minimal losses to the cam on the source side by the compression of the rods during the binding of the target molecule to the receptor, a process that regenerates mechanical energy. The artificial receptors are best designed for high affinity binding in the presence of a dominant background of quite different molecules. Analogies with antibodies suggest that a rotor with binding pockets of this type could deliver a product stream with impurity fractions on the order of 10^{-4} to 10^{-9} (i.e., 99.99% purity or better) depending on affinities, specificities, and the concentrations of the effectively competing ligands.[25] A detailed computational modeling and simulation effort will be required to create ideal selective binding site designs for CO_2 and also for additional specific target molecules of interest including CO, NO_x, and UHC.



However, even an extremely simple binding site may be surprisingly effective. The figure at left[26] is an example of a very simple 420-atom binding site (C = black, H = white, O = red) that does not employ strong covalent bonds between the site and the target molecule. This binding site was designed by taking a thin sheet of hydrogen-terminated lonsdaleite (aka. hexagonal diamond) with the C(111) lattice on the top and bottom horizontal faces, cutting out a hexagonal perimeter with the C(100) lattice on all six vertical sides, punching a small hole in the center, and hydrogenating the inner walls of the pore, making a 420-atom ($C_{240}H_{180}$) all-hydrocarbon binding site. Such a structure could readily be nanofabricated as a solid block using a specific sequence of positionally-controlled tip-based mechanosynthetic reactions.[27] The image (left) shows a single CO_2 molecule (image, right) nestled snugly inside the hydrogen-terminated pore, which employs only van der Waals attractions to provide the necessary binding interaction.

In a previously published assessment of the molecular selectivity of this simple CO_2 binding site,[28] we listed 38 major and trace atmospheric constituents typically found in non-urban air

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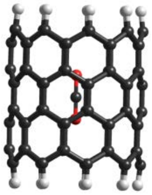
[25] Drexler KE. Nanosystems: Molecular Machinery, Manufacturing, and Computation. John Wiley & Sons, New York, 1992, Section 13.2.2(b); https://www.amazon.com/dp/0471575186/.

[26] Design by Ralph C. Merkle; personal communication, 2015.

[27] e.g., Freitas RA Jr, Merkle RC. A Minimal Toolset for Positional Diamond Mechanosynthesis. J Comput Theor Nanosci. 2008 May;5:760-861; http://www.molecularassembler.com/Papers/MinToolset.pdf.

along with their fractional molar concentration,[29] then employed molecular mechanics methods using the AMBER99 force field[30] (known to be highly parameterized for nonbonded interactions, using the computational tools of quantum chemistry) to estimate the binding energy (E_b) of the pore for each molecular species (Table 3, below). This was calculated as the difference between the total energy of the binding site with the molecule bound inside it and the sum of the total energies of the empty binding site and the isolated molecule. The fractional binding site occupancy of a molecular species, or $\exp(-E_b/k_B T)$ where $k_B = 8.625 \times 10^{-5}$ eV/molecule-K and ambient temperature T = 300 K, was then multiplied by the fractional atmospheric molar concentration (f_{air}) of that molecule, then renormalized to obtain the percentage of each molecular species likely to be captured by the binding site in the first pass. This competitive affinity analysis concluded that the proposed simple binding site has very high affinity for CO_2 and even higher affinity for eight other molecules, but those other eight molecules are present in normal air at such low concentrations that the resulting gaseous filtrate is ~99% pure CO_2, with just ~1% of O_2 and N_2 and mere traces of everything else.[31] This analysis assumed a temperature of T = 300 K but the relative affinities and selectivities should not substantially change at T ~ 573 K (300 °C).



The 420-atom binding site design presented here is offered as just one example of a wide range of possibilities. An even simpler binding site based on the CNT(9,0) carbon nanotube (image, left),[32] similarly evaluated using AMBER, appears to prefer CO_2 (-0.73 eV) over SO_2 (-0.62 eV), with additional binding energies of -0.49 eV (O_2), -0.45 eV (CO), -0.35 eV (H_2O), -0.33 eV (N_2), and -0.06 eV (H_2).

Note that the onboard filter is deliberately designed not to capture water in the car, which would waste rotor effort and onboard storage space. The water is recaptured later (Section 6.1).

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[28] Freitas RA Jr. The Nanofactory Solution to Global Climate Change: Atmospheric Carbon Capture. IMM Report No. 45, December 2015; http://www.imm.org/Reports/rep045.pdf.

[29] Killinger DK, Churnside JH, Rothman LS. Chapter 44. Atmospheric Optics. Bass M, Van Stryland EW, Williams DR, Wolfe WL, eds., Handbook of Optics, Volume I: Fundamentals, Techniques, and Design, Second Edition, McGraw-Hill, Inc., New York, 1995, pp. 44.1-44.50. Weast RC, Handbook of Chemistry and Physics, 49th Edition, CRC, Cleveland OH, 1968.

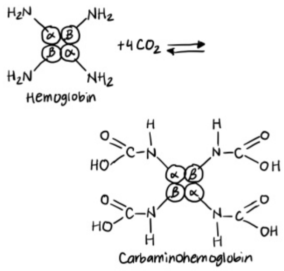
[30] Cornell WD, Cieplak P, Bayly CI, Gould IR, Merz KM Jr, Ferguson DM, Spellmeyer DC, Fox T, Caldwell JW, Kollman PA. A second generation force field for the simulation of proteins, nucleic acids, and organic molecules. J Am Chem Soc. 1995;117: 5179-5197; http://homepage.univie.ac.at/mario.barbatti/papers/method/amber_1995.pdf. Wang J, Cieplak P, Kollman PA. How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules? J Comput Chem. 2000;21(12):1049-1074; http://banana.cnsm.csulb.edu/ffamber/pdfs/wang_amber99_2000jcc.pdf.

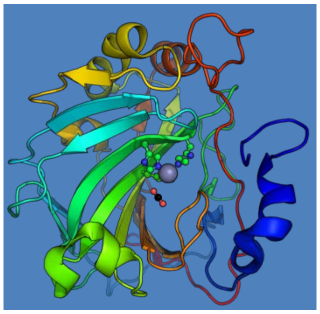
[31] Filtrate purity will vary slightly with ambient environmental temperature (e.g., 99.26% CO_2 at 290 K, 98.49% CO_2 at 310 K). Note also that a single-stage filter of this type applied to flue gas from a coal-fired power plant would produce filtrate gas containing 52% CO_2 and 48% SO_2; applying a second stage of the same filters to the first-stage filtrate would extract essentially all of the SO_2, since the second-stage filtrate would be 99.6% SO_2 and 0.4% CO_2. Filters can be cascaded if necessary.

[32] Design by Ralph C. Merkle; personal communication, 2015.

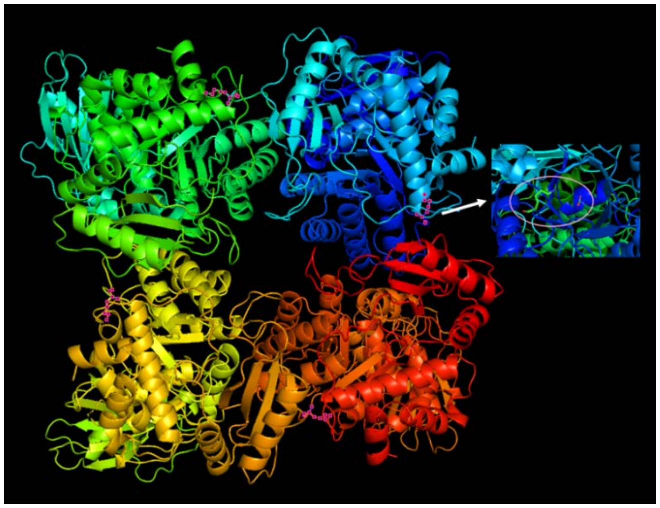
Table 3. Gas molecule concentrations in ambient U.S. dry atmosphere, their binding energy in the proposed binding site assuming T = 300 K, and their concentrations in the resulting filtrate.

Atmospheric Molecular Component	Fractional Atmospheric Concentration (f_{air})	Amber99 Binding Energy of Molecular Component in Simple Binding Site (E_b)	% Concentration of Air Component in Gas Filtrate
Nitrogen (N_2)	7.80840 x 10^{-1}	-0.2521 eV	0.1386%
Oxygen (O_2)	2.09460 x 10^{-1}	-0.3336 eV	0.8665%
Water vapor (H_2O)	~1.00 x 10^{-2}	-0.2936 eV	0.0088%
Argon (Ar)	9.340 x 10^{-3}	-0.0586 eV	< 1 ppm
Carbon Dioxide (CO_2)	3.870 x 10^{-4}	-0.6190 eV	98.9341%
Neon (Ne)	1.818 x 10^{-5}	-0.1021 eV	< 1 ppm
Helium (He)	5.24 x 10^{-6}	-0.0535 eV	< 1 ppm
Methane (CH_4)	1.79 x 10^{-6}	-0.3210 eV	< 1 ppm
Krypton (Kr)	1.14 x 10^{-6}	-0.0904 eV	< 1 ppm
Hydrogen (H_2)	5.50 x 10^{-7}	-0.0461 eV	< 1 ppm
Nitrous Oxide (N_2O)	3.20 x 10^{-7}	-0.4611 eV	0.0002%
Carbon Monoxide (CO)	1.50 x 10^{-7}	-0.2999 eV	< 1 ppm
Xenon (Xe)	8.70 x 10^{-8}	-0.1028 eV	< 1 ppm
Ozone (O_3)	2.66 x 10^{-8}	-0.6287 eV	0.0099%
Formaldehyde (H_2CO)	2.4 x 10^{-9}	-0.5542 eV	0.0001%
Ethane (C_2H_6)	2.0 x 10^{-9}	-0.6816 eV	0.0058%
Hydrogen Chloride (HCl)	1.0 x 10^{-9}	-0.3833 eV	< 1 ppm
Methyl Chloride (CH_3Cl)	7.0 x 10^{-10}	-0.6842 eV	0.0022%
Carbonyl Sulfide (OCS)	6.0 x 10^{-10}	-0.7324 eV	0.0123%
Acetylene (C_2H_2)	3.0 x 10^{-10}	-0.5079 eV	< 1 ppm
Sulfur Dioxide (SO_2)	3.0 x 10^{-10}	-0.7650 eV	0.0216%
Nitric Oxide (NO)	3.0 x 10^{-10}	-0.3052 eV	< 1 ppm
Hydrogen Peroxide (H_2O_2)	2.0 x 10^{-10}	-0.4974 eV	< 1 ppm
Hydrogen Cyanide (HCN)	1.7 x 10^{-10}	-0.5523 eV	< 1 ppm
Nitric Acid (HNO_3)	5.0 x 10^{-11}	-0.4311 eV	< 1 ppm
Ammonia (NH_3)	5.0 x 10^{-11}	-0.1887 eV	< 1 ppm
Nitrogen Dioxide (NO_2)	2.3 x 10^{-11}	-0.5395 eV	< 1 ppm
Hypochlorous Acid (HOCl)	7.7 x 10^{-12}	-0.5970 eV	< 1 ppm
Hydrogen Iodide (HI)	3.0 x 10^{-12}	-0.4993 eV	< 1 ppm
Hydrogen Bromide (HBr)	1.7 x 10^{-12}	-0.4707 eV	< 1 ppm
Hydroxyl radical (OH^-)	4.4 x 10^{-14}	-0.3443 eV	< 1 ppm
Hydrogen Fluoride (HF)	1.0 x 10^{-14}	-0.2439 eV	< 1 ppm
Chlorine Monoxide (ClO)	1.0 x 10^{-14}	-0.6515 eV	< 1 ppm
Formic Acid (HCOOH)	1.0 x 10^{-14}	-0.7281 eV	< 1 ppm
Carbonyl Fluoride (COF_2)	1.0 x 10^{-14}	-0.3756 eV	< 1 ppm
Sulfur Hexafluoride (SF_6)	1.0 x 10^{-14}	0.3578 eV	< 1 ppm
Hydrogen Sulfide (H_2S)	1.0 x 10^{-14}	-0.3699 eV	< 1 ppm
Phosphine (PH_3)	1.0 x 10^{-20}	-0.4062 eV	< 1 ppm





In the biological world, many proteins and enzymes have binding sites for carbon dioxide. For example, hemoglobin reversibly binds CO_2, forming carbamino hemoglobin (image, right).[33] A zinc enzyme present in red blood cells, carbonic anhydrase,[34] catalyzes the hydration of dissolved carbon dioxide to bicarbonate ion, so this enzyme (a CO_2 is visible near center of image at left)[35] has receptors for both CO_2 and H_2O. The first step in chlorophyllic photosynthesis, in which CO_2 is added to a 5-carbon sugar, is catalyzed by ribulose biphosphate carboxylase (image, below),[36] probably the world's most abundant enzyme because it accounts for more than half the soluble protein in every green leaf on Earth.[37] (This enzyme effectively has two separate CO_2 binding sites, along with a third oxygenase site that binds O_2.[38])



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[33] https://en.wikipedia.org/wiki/Carbaminohemoglobin.

[34] Devlin TM, ed. Textbook of Biochemistry with Clinical Correlations. John Wiley & Sons, New York, 1986; https://www.amazon.com/Textbook-Biochemistry-Clinical-Correlations-publication/dp/0471814628/.

[35] https://en.wikipedia.org/wiki/Carbonic_anhydrase.
[36] https://en.wikipedia.org/wiki/RuBisCO.

[37] Zubay G. Biochemistry, Second Edition. Macmillan, New York, 1988; https://www.amazon.com/Biochemistry-2ND-Geoffrey-Zubay/dp/B000O8QNJU/.

[38] Stec B. Structural mechanism of RuBisCO activation by carbamylation of the active site lysine. Proc Natl Acad Sci U S A. 2012 Nov 13;109(46):18785-90; https://www.pnas.org/content/109/46/18785. Van Lun M, Hub JS, van der Spoel D, Andersson I. CO_2 and O_2 distribution in Rubisco suggests the small subunit functions as a CO_2 reservoir. J Am Chem Soc. 2014 Feb 26;136(8):3165-71; http://cmb.bio.uni-goettingen.de/pub/VanLun_JACS2014.pdf or https://biophys.uni-saarland.de/pub/VanLun_JACS2014.pdf.

5. Compression of Retained Exhaust Gases

The retained exhaust gases are ($M_{CO2filter}$ / $M_{compress}$ ~) 96.5% carbon dioxide, which becomes a supercritical fluid when compressed to 1000 atm depending on temperature.[39] This fluid reaches a density of $\rho_{CO2,1000atm}$ ~ 700 kg/m^3 at 573 K (300 °C),[40] requiring a total onboard high pressure storage volume of $V_{1000atm}$ ~ $M_{compress}$ / $\rho_{CO2,1000atm}$ ~ 0.20 m^3. (The remaining ~3.5% of mixed gases in the exhaust stream are assumed for computational convenience to be of roughly comparable compressibility and chemically unreactive when compressed to 1000 atm.) A pressure vessel of this volume would represent only $V_{1000atm}$ / V_{car} ~ 1% of the total displaced volume of a 5 m x 2 m x 1.5 m sedan with V_{car} ~ 15 m^3.

A single spherical pressure vessel of volume $V_{1000atm}$ and radius $R_{vessel} = (3\ V_{1000atm} / 4\pi)^{1/3}$ = 36.0 cm with wall material of working strength $\sigma_w \sim 10^{10}$ N/m^2 (as a conservative value for atomically precise flawless monocrystalline diamond of density $\rho_{diamond}$ = 3510 kg/m^3)[41] intended to restrain a fluid pressure of p_{fluid} (= 1000 atm = 1.01 x 10^8 N/m^2) without bursting requires a minimum vessel wall thickness[42] of $x_{wall} \geq p_{fluid}\ R_{vessel} / 2\ \sigma_w$ ~ 1.8 mm, producing an empty vessel mass of at least $M_{vessel} = 4\pi\ R_{vessel}^2\ x_{wall}\ \rho_{diamond}$ = 10.3 kg. If a nonspherical form factor is desired for the pressure vessel, the storage volume can be divided into multiple smaller closely-packed spheres that fill space with a ~68% packing density,[43] increasing total vessel volume by $0.68^{-1} - 1$ ~ 47%, but which can conveniently be arranged in a container shape having any desired form factor with the same total vessel mass – e.g., a system using 1000 small spherical vessels each of radius 3.6 cm and wall thickness 0.18 mm. Some additional material mass and volume will be required for the physical infrastructure needed to support and operate the onboard pressure vessel. Handling a pressure vessel at 300 °C on a vehicle might be considered challenging, but the vessel and pumps would be designed to dissipate heat quickly.

The energy cost of isothermally[44] compressing CO$_2$ from an initial pressure of $p_1 = p_{exhaust}$ ($M_{CO2filter}$ / $M_{tailpipe}$) ~ 0.2 atm[45] to p_2 = 1000 atm at a temperature of T_{gas} = 573 K (300 °C) with

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[39] https://en.wikipedia.org/wiki/Carbon_dioxide#/media/File:Carbon_dioxide_pressure-temperature_phase_diagram.svg.

[40] https://www.engineeringtoolbox.com/carbon-dioxide-density-specific-weight-temperature-pressure-d_2018.html.

[41] We choose diamond (or similarly strong nanoengineered materials) because the vessel walls would be thicker and heavier by an order of magnitude using conventional high-strength alloys (e.g., ~1 GPa).

[42] Freitas RA Jr. Nanomedicine, Volume I: Basic Capabilities. Landes Bioscience, Georgetown, TX, 1999, Section 10.3.1, “Fluid Storage Tank Scaling”; http://www.nanomedicine.com/NMI/10.3.1.htm.

[43] Gasson PC. Geometry of Spacial Forms, John Wiley & Sons, New York, 1983; https://www.amazon.com/Geometry-Spatial-Horwood-Mathematics-Applications/dp/0853126208/.

[44] Isothermal compression is the minimal work scenario. If compression was adiabatic, for an ideal gas the energy cost is a little over twice the isothermal figure, or $W \sim [(R_{specificCO2}\ T_{gas}) / \gamma - 1)]\ [(p_2 / p_1)^{((\gamma-1)/\gamma)} - 1]$ = 2.22 MJ/kg, taking the heat capacity ratio $\gamma \sim 1.3$ for CO$_2$. In this application, the compression process

CO_2 specific gas constant $R_{specificCO2}$ = 189 J/kg-K is $E_{CO2,1000atm} \sim R_{specificCO2}\, T_{gas} \ln(p_2/p_1)$ = 922 kJ/kg, taking $p_{exhaust} \sim 1$ atm (normal engine exhaust pressure). Therefore the approximate energy cost to compress the retained exhaust gases is $E_{compress} = E_{CO2,1000atm}\, M_{compress} \sim 130$ MJ, or an average power consumption of $P_{compress} = E_{compress} / t_{drive}$ = **5.5 kW** if the car is operated continuously in typical highway or city driving.

Together, the molecular sortation system (Section 3) and the retained exhaust gas compression system (Section 5) draw $P_{storage} = P_{rotors} + P_{compress} \sim 9.3$ kW of available onboard gasoline-sourced vehicular power.

Molecular motors and powerplants fabricated via atomically precise manufacturing can have significantly higher efficiencies than the $\varepsilon_{car} \sim 25\%$ typically achieved by internal combustion engines in cars. For example, the RNA polymerase[46] and actomyosin[47] molecular motors convert chemical into mechanical energy with ~40% and ~60% efficiency, respectively, and the bacterial flagellar proton gradient chemomechanical motor achieves 50-99% efficiency at high load.[48] Drexler[49] estimates from first principles that chemically-driven engines can be designed to operate at >99% efficiency at a power density of $\sim 10^9$ watts/m^3. Even if the chemical energy stored in gasoline could be converted into mechanical energy for molecular sortation and gas compression with an efficiency of only $\varepsilon_{APM} \sim 50\%$,[50] then properly outfitted zero-emission cars

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can be made very close to isothermal because of the exceptionally high thermal conductivity of the monocrystalline flawless diamond of which the pumping mechanisms and storage tanks holding the CO_2 are constructed, enabling rapid removal of the heat generated during compression. This rapid heat dissipation helps maintain a nearly constant temperature during the compression process – in essence, the diamond components act like built-in, highly efficient intercoolers, mitigating the temperature rise and reducing the work input needed.

[45] 0.2 atm is the effective partial pressure of CO_2 in the exhaust gas.

[46] Freitas RA Jr. Nanomedicine, Volume I: Basic Capabilities. Landes Bioscience, Georgetown, TX, 1999, Section 6.3.4.2, "Biological Chemomechanical Power Conversion"; http://www.nanomedicine.com/NMI/6.3.4.2.htm.

[47] Spudich JA. How molecular motors work. Nature. 1994 Dec 8;372(6506):515-8; http://lilith.fisica.ufmg.br/~dickman/transfers/qbio/motors/howdomolecularmotorswork.pdf.

[48] Jones CJ, Aizawa S. The bacterial flagellum and flagellar motor: structure, assembly and function. Adv Microb Physiol. 1991;32:109-72; https://pubmed.ncbi.nlm.nih.gov/1882727/.

[49] Drexler KE. Nanosystems: Molecular Machinery, Manufacturing, and Computation. John Wiley & Sons, New York, 1992, Section 13.3.8, "Mechanochemical power generation"; https://www.amazon.com/dp/0471575186/.

[50] Note that the highest energy efficiency achieved in a gasoline-powered internal combustion engine is around 50% (thermal efficiency), and this has been demonstrated in Formula 1 hybrid engines such as those used by Mercedes-AMG and Honda F1 power units in the turbo-hybrid era since 2014. See: Lawrence Butcher, "The best engine that will ever exist? Ultimate efficiency of F1's hybrid. 135 years of innovation: making of the internal combustion engine, Part 8." MotorSport, 21 Feb 2022; https://www.motorsportmagazine.com/articles/racing-tech/the-best-engine-that-will-ever-exist-ultimate-efficiency-of-f1s-hybrid/. Hazel Southwell, "How F1 can push "the world's most efficient engine" even

would consume just $t_{drive}\ P_{storage}\ /\ \varepsilon_{APM}\ E_{gasoline}$ ~ 21% of the chemical energy stored in 16 gallons of gasoline to achieve zero emissions, leaving 79% of the chemical energy stored in the gasoline available to power physical motion of the vehicle in the normal manner, via combustion. Even this modest requirement is easily offset by simply adding another ~3 gallons of fuel capacity to the gas tank.

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further." RaceFans, 11 Nov 2021; https://www.racefans.net/2021/11/11/how-f1-can-push-the-worlds-most-efficient-engine-even-further/.

6. Gasoline Service Stations

In the scenario presented here, a passenger car leaves a local gasoline service station having filled its 16 gallon tank full of gasoline (e.g., taken here as pure octane[51] or C_8H_{18}) of fluid mass $M_{gasoline}$ ~ 44.2 kg (60.6 L). Its onboard pressure vessel is empty (0 kg of contained fluid). The car is then driven as a standard internal combustion vehicle, with the gasoline burned using inhaled oxygen drawn from the external atmospheric environment. During operation, the car emits through its tailpipe only the remnant exhaust gases (mostly nitrogen gas and water vapor), 99.998% of which are naturally present in the atmosphere (Table 2). After a period of operation, the car pulls into a second gasoline service station, in the most extreme case just as its gasoline tank reaches empty. The car's gas tank now contains 0 kg of gasoline and its onboard pressure vessel has been filled with $M_{compress}$ = 141.4 kg of remnant exhaust gases compressed to 1000 atm with the approximate composition listed in Table 2 (Section 2). The car weighs $\Delta M = M_{compress} - M_{gasoline}$ ~ 97.2 kg more at the end of its journeys than at the beginning – roughly the weight of one very stocky human passenger (~214 lbs) representing an increase of only $\Delta M / M_{car}$ ~ 5% in the total weight of an average car of mass M_{car} ~ 1860 kg.[52] The car offloads its compressed remnant exhaust gases into a service station receptacle, refills its tank with 16 gallons of fresh gasoline, pays the station for the transaction, then resumes its zero-emission journeys with its now-empty onboard pressure vessel.

Following this transaction, the station receptacle contains the remnant exhaust gas components compressed to p_2 = 1000 atm pressure at the approximate partial pressures listed in Table 4, assuming $p_n \sim (M_n / M_{compress})\, p_2$ for gas component n.

Table 4. Approximate partial pressure of remnant exhaust gases delivered to the service station receptacle.

Mixed Exhaust Component	**Mass (kg)**	**p_n (atm)**	**Mixed Exhaust Component**	**Mass (kg)**	**p_n (atm)**
Combustion CO_2	136.5	965.4	Atmospheric N_2	0.0	0.0
Combustion H_2O	0.0	0.0	Atmospheric Ar	0.0	0.0
Combustion CO	3.992	28.3	Atmospheric H_2O	0.0	0.0
Combustion NO_x	0.3992	2.8	Atmospheric CO_2	0.0	0.0
Combustion UHC	0.499	3.5	***Total*** ($M_{compress}$)	***141.4***	*1000.0*

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[51] https://en.wikipedia.org/wiki/Octane.

[52] https://www.autolist.com/guides/average-weight-of-car.

6.1 Acquire Atmospheric Water

The service station employs an array of atmosphere-facing sorting rotors equipped with high-affinity binding sites for water molecules to absorb from ambient air the entire M_{H2O} ~ 62.8 kg of H_2O that were previously released into the atmosphere by the car during its travels (Table 2) and will be needed in subsequent chemical processing for octane regeneration (see below). This recapture of water completes the H_2O cycle and satisfies the objective of zero net emissions of water from the moving vehicle.

A few binding sites are known for H_2O molecules but more research is needed in this area. For example, helical transmembrane proteins acquire "buried water" in internal voids,[53] and a lithium-organic framework[54] and the five-coordinate, square-pyramidal *trans*-$RuCl_2(P–N)(PPh_3)$ complex[55] reversibly bind water. Various materials also form 3D networks that can reversibly bind crystallization water molecules,[56] and many molecules bind water reversibly such as deliquescent crystals, efflorescent minerals, hydrophilic and polar amino acids, and numerous enzymes such as carbonic anhydrase, hydrolases and dehydratases.[57] Binding sites for frozen water-ice are also known.[58]

Using sorting rotors to concentrate M_{H2O} ~ 62.8 kg of atmospheric H_2O from a partial pressure of p_{atmH2O} ~ 0.0025 atm to a pressure of p_{atm} ~ 1 atm has an energy cost of $E_{atmH2O} \sim (M_{H2O}\ N_A / MW_{H2O})\ k_B T \ln(p_{atm}/p_{atmH2O}) = 52.2$ MJ, taking $MW_{H2O} = 0.018$ kg/mole and T = 300 K at the service station. We must extract $n_{H2O} = M_{H2O}\ N_A / MW_{H2O} = 2.10 \times 10^{27}$ molecules of H_2O, requiring a maximum of $N_{rotorsH2O} = n_{H2O} / r_{sort}\ t_{service} = 4.86 \times 10^{18}$ sorting rotors of total mass $M_{rotorsH2O} \sim M_{rot}\ N_{rotorsH2O} = 9.72$ gm, total volume $V_{rotorsH2O} \sim V_{rot}\ N_{rotorsH2O} = 6.67\ cm^3$, and

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[53] Renthal R. Buried water molecules in helical transmembrane proteins. Protein Sci. 2008 Feb;17(2):293-8; https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2222723/.

[54] El Osta R, Frigoli M, Marrot J, Guillou N, Chevreau H, Walton RI, Millange F. A lithium-organic framework with coordinatively unsaturated metal sites that reversibly binds water. Chem Commun (Camb). 2012 Nov 7;48(86):10639-41; https://pubmed.ncbi.nlm.nih.gov/23001396/.

[55] Ma ES, Patrick BO, James BR. Reversible binding of water, methanol, and ethanol to a five-coordinate ruthenium(II) complex. Dalton Trans. 2013 Mar 28;42(12):4291-8; https://pubmed.ncbi.nlm.nih.gov/23344393/.

[56] Zheng Y, Kustaryono D, Kerbellec N, Guillou O, Gérault Y, Le Dret F, Daiguebonne C. The lanthanide-containing cyclohexane-tri-carboxylate coordination polymers re-investigated," Inorganica Chimica Acta 2009 May 15;362(7):2123-2126; https://www.sciencedirect.com/science/article/abs/pii/S002016930800604X.

[57] Devlin TM, ed. Textbook of Biochemistry with Clinical Correlations. John Wiley & Sons, New York, 1986; https://www.amazon.com/Textbook-Biochemistry-Clinical-Correlations-publication/dp/0471814628/.

[58] Hudait A, Qiu Y, Odendahl N, Molinero V. Hydrogen-Bonding and Hydrophobic Groups Contribute Equally to the Binding of Hyperactive Antifreeze and Ice-Nucleating Proteins to Ice. J Am Chem Soc. 2019 May 15;141(19):7887-7898; https://par.nsf.gov/servlets/purl/10092995.

maximum power consumption $P_{rotorsH2O} = P_{rot}\ N_{rotorsH2O}$ = 224 kW, taking the extraction time as equal to the time allotted to service each car, or $t_{service}$ ~ 432 sec/car (Section 7).

6.2 Metabolize Compressed CO_2 and Regenerate Octane (gasoline)

Octane is regenerated using CO_2 stored in the station receptacle and H_2O sourced from the atmosphere by applying at least $E_{gasoline}$ ~ 2120 MJ of energy to force the combustion reaction previously described in Section 2 to proceed endoergically "uphill" in energy using atomically precise manufacturing techniques including mechanosynthesis,[59] as:

$$E_{octane} + 16\ CO_2 + 18\ H_2O \rightarrow 2\ C_8H_{18}\ \text{(octane)} + 25\ O_2$$
$$16\ (0.044\ \text{kg/mole}) + 18\ (0.018\ \text{kg/mole}) \rightarrow 2\ (0.114\ \text{kg/mole}) + 25\ (0.032\text{kg/mole})$$
$$0.704\ \text{kg}\ CO_2 + 0.324\ \text{kg}\ H_2O \rightarrow 0.228\ \text{kg}\ C_8H_{18} + 0.8\ \text{kg}\ O_2$$
$$136.5\ \text{kg}\ CO_2 + 62.8\ \text{kg}\ H_2O \rightarrow 44.2\ \text{kg}\ C_8H_{18} + 155.1\ \text{kg}\ O_2$$

Assuming the regeneration reaction can be made $\varepsilon_{mechanochem}$ ~ 50% efficient,[60] then the energy cost of octane synthesis is $E_{octane} \sim E_{gasoline} / \varepsilon_{mechanochem}$ ~ 4240 MJ, less the energy recoverable from the decompression of the CO_2 from a partial pressure of $p_{CO2,compress}$ = 965.4 atm (Table 4) to p_{atm} = 1 atm, or $E_{CO2,decompress} \sim M_{CO2}\ R_{specificCO2}\ T_{gas}\ \ln(p_{CO2,compress} / p_{atm})$ = 53.2 MJ, taking T_{gas} ~ 300 K. This gives a net energy cost of octane regeneration of $E_{octane,net} = E_{octane} - E_{CO2,decompress}$ ~ 4190 MJ to produce 44.2 kg of octane (~gasoline), along with 155.1 kg of molecular oxygen gas which is released back into the atmosphere, completing the oxygen cycle and satisfying the objective of zero net atmospheric alterations due to the moving vehicle.

6.3 Metabolize Compressed CO and UHC

The techniques of mechanosynthesis can also be employed at the service station to convert the unwanted carbon monoxide (CO) and unburned hydrocarbons (represented here by propylene (C_3H_6) as a reasonable proxy for the effective $C_{3.325}H_{6.6}O_{0.025}$ "average hydrocarbon" estimated

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[59] Freitas RA Jr. Cell Mills: Nanofactory Manufacture of Biological Components. IMM Report No. 53, 15 June 2024; Section 2.1.2, "Molecular Manufacturing of Generic Organics"; http://www.imm.org/Reports/rep053.pdf.

[60] Freitas RA Jr. Cell Mills: Nanofactory Manufacture of Biological Components. IMM Report No. 53, 15 June 2024; Section 2.1.2.2, "Quantitative Productivity of Generic Synthesis Unit"; http://www.imm.org/Reports/rep053.pdf. Note that the efficiency of the Sabatier reaction process ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$), including electrolysis of water to obtain the H_2, has recently been reported as high as 76% in an operating industrial system (Moioli E, Senn P, Østrup S, Hütter C. Results from the operation of an efficient and flexible large-scale biogas methanation system. Energy Adv. 2024;3:131-142; https://pubs.rsc.org/en/content/articlehtml/2024/ya/d3ya00436h), and the synthesis of long-chain hydrocarbons from carbon oxides can have a thermal efficiency of 50% using the Fischer-Tropsch process (https://en.wikipedia.org/wiki/Fischer%E2%80%93Tropsch_process#Process_efficiency) and 60% for the Syngas-to-Gasoline process (https://en.wikipedia.org/wiki/Syngas_to_gasoline_plus#Process_efficiency).

earlier in Section 2) into useful additional octane (for use as fuel) and molecular oxygen (for release into the atmosphere), which may be approximated by the following reactions:

$$E_{CO} + 142.9\ CO \rightarrow 71.45\ O_2 + 142.9\ C$$
$$4.00\ kg\ CO \rightarrow 2.29\ kg\ O_2 + 1.71\ kg\ C$$

and

$$E_{UHC} + 11.9\ C_3H_6 \rightarrow 3.97\ C_8H_{18}\ (\text{octane}) + 4\ C$$
$$0.5\ kg\ C_3H_6 \rightarrow 0.452\ kg\ C_8H_{18} + 0.048\ kg\ C$$

with E_{CO} = 0 – (142.9 moles) ΔH°f (CO) = 15.8 MJ (an endothermic process, so energy must added) and E_{UHC} = (3.97 moles) ΔH°f (C_8H_{18}) – (11.9 moles) ΔH°f (C_3H_6) = -1.2 MJ (a net exothermic process, so energy is generated), taking ΔH°f (CO) = -110.5 kJ/mole, ΔH°f (C_3H_6) = +20.4 kJ/mole, and ΔH°f (C_8H_{18}) = -250 kJ/mole. The total energy input is approximately $E_{CO+UHC} = (E_{CO} + E_{UHC}) / \varepsilon_{mechanochem}$ ~ 29.2 MJ, less the energy recoverable from the decompression of the CO and UHC from a combined partial pressure of $p_{CO+UHC,compress}$ = 31.8 atm to p_{atm} = 1 atm, or $E_{CO+UHC,decompress} \sim (M_{CO} + M_{UHC})\ R_{specificCO+UHC}\ T_{gas}\ \ln(p_{CO+UHC,compress} / p_{atm})$ = 1.3 MJ, taking T_{gas} ~ 300 K and specific gas constant $R_{specificCO+UHC}$ ~ 286 J/kg-K. This gives a net energy cost of CO and UHC metabolization of $E_{CO+UHC,net} \sim E_{CO+UHC} - E_{CO+UHC,decompress}$ = 27.9 MJ to produce 0.452 kg of octane, 1.758 kg of pure carbon (which can be collected for reuse),[61] and 2.29 kg of molecular oxygen gas which is released back into the atmosphere.

We must extract $n_{CO} = M_{CO}\ N_A / MW_{CO} = 8.60 \times 10^{25}$ molecules of CO and $n_{UHC} = M_{UHC}\ N_A / MW_{UHC} = 6.27 \times 10^{24}$ molecules of UHC from the compressed exhaust gases, taking MW_{CO} = 0.028 kg/mole and MW_{UHC} = 0.048 kg/mole. This requires a maximum of $N_{rotorsCO+UHC} = (n_{CO} + n_{UHC}) / r_{sort}\ t_{service} = 2.14 \times 10^{17}$ sorting rotors of total mass $M_{rotorsCO+UHC} \sim M_{rot}\ N_{rotorsCO+UHC}$ = 0.428 gm, total volume $V_{rotorsCO+UHC} \sim V_{rot}\ N_{rotorsCO+UHC} = 0.294\ cm^3$, and maximum power consumption $P_{rotorsCO+UHC} = P_{rot}\ N_{rotorsCO+UHC}$ = 9.8 kW, taking $t_{service}$ ~ 432 sec/car.

6.4 Metabolize Compressed NO_x

Mechanosynthesis can additionally be employed at the service station to convert the unwanted nitrogen oxides, e.g., nitric oxide (NO), into harmless molecular nitrogen (N_2) and oxygen (O_2) for release into the atmosphere, as approximated by the following reaction:

$$13.3\ NO \rightarrow 6.7\ N_2 + 6.7\ O_2 + E_{NOx}$$
$$0.4\ kg\ NO \rightarrow 0.19\ kg\ N_2 + 0.21\ kg\ O_2$$

with E_{NOx} = 0 – (13.3 moles) ΔH°f (NO) = -1.2 MJ (a net exothermic process, so energy is generated), taking ΔH°f (NO) = +90.7 kJ/mole. The total energy generated is approximately $E_{NO} = E_{NO}\ \varepsilon_{mechanochem}$ ~ 0.6 MJ, plus the energy recoverable from the decompression of the NO from a partial pressure of $p_{NO,compress}$ = 2.8 atm to p_{atm} = 1 atm, or $E_{NO,decompress} \sim M_{NO}\ R_{specificNO}\ T_{gas}\ \ln(p_{NO,compress} / p_{atm})$ = 0.3 MJ, taking T_{gas} ~ 300 K and specific gas constant $R_{specificNO}$ ~ 277 J/kg-

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[61] Improved engine design, likely benefiting from atomically precise manufacturing, could greatly reduce CO and UHC formation, minimizing carbon loss each cycle.

K. This gives a negligible net energy generation of $E_{NO,net} \sim E_{NO} - E_{NO,decompress} = 0.9$ MJ to produce 0.19 kg of molecular nitrogen gas and 0.21 kg of molecular oxygen gas, both of which are harmlessly released back into the atmosphere.

We must extract $n_{NOx} = M_{NOx} N_A / MW_{NOx} = 8.03 \times 10^{24}$ molecules of NO_x from the compressed exhaust gases, taking $MW_{NOx} = 0.030$ kg/mole. This requires a maximum of $N_{rotorsNOx} = n_{NOx} / r_{sort} t_{service} = 1.86 \times 10^{16}$ sorting rotors of total mass $M_{rotorsNOx} \sim M_{rot} N_{rotorsNOx} = 0.037$ gm, total volume $V_{rotorsNOx} \sim V_{rot} N_{rotorsNOx} = 0.026 \text{ cm}^3$, and maximum power consumption $P_{rotorsNOx} = P_{rot} N_{rotorsNOx} = 0.9$ kW, taking $t_{service} \sim 432$ sec/car.

6.5 Service Station Summary

Replenishing the 16 gallons of gasoline needed by one car at the service station thus requires +52.2 MJ to acquire atmospheric water (Section 6.1), +4190 MJ to metabolize the compressed CO_2 and synthesize octane (Section 6.2), and +27.9 MJ to metabolize the compressed CO and UHC into octane, O_2 and carbon (Section 6.3), and generates -1.5 MJ while metabolizing the compressed NO_x into N_2 and O_2 (Section 6.4), for a net energy cost of $E_{fillup} = +4270$ MJ to service one automobile. Taking $K_{elect} = \$0.1285$/kW-hr as the average cost of commercial electricity in 2024,[62] the cost of this energy today would be $C_{fillup} = K_{elect} E_{fillup} = \$152$, equivalent to $C_{fillup} / V_{tank} \sim$ **\$9.50/gallon of gasoline**. However, if as expected the price of electricity falls significantly by the time this scheme is implemented – e.g., if the cost of electricity has fallen 100-fold to ~\$0.001/kW-hr using solar panels manufactured using nanofactories[63] – then the cost of a 16-gallon fillup could fall to ~\$1.19, equivalent to ~**\$0.07/gallon gasoline**.

Following previously published estimates,[64] a Generic Synthesis Unit specialized for small molecule synthesis with nanomachinery mass $M_{FSB} \sim 73$ gm and volume $V_{FSB} \sim 36.5 \text{ cm}^3$ could synthesize small molecules like octane at a production rate of $R_{CellMill} \sim 24$ kg/day. Servicing $N_{cars} = 200$ cars/day thus requires a fairly modest nanomachinery synthesis plant of mass $M_{synth} = (M_{FSB} / R_{CellMill}) (N_{cars} M_{gasoline}) = 27$ kg and volume $V_{synth} = (V_{FSB} / R_{CellMill}) (N_{cars} M_{gasoline}) = 0.0134 \text{ m}^3$, along with one or more ~0.20 m^3 station receptacles at each service station. For comparison, modern-day gas stations typically employ one or more underground gasoline storage tanks ranging from 10,000-20,000 gallons (38-76 m^3) in volume.[65]

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[62] EIA, Table 5.3 Average Price of Electricity to Ultimate Customers. Electric Power Monthly, Feb 2025; https://www.eia.gov/electricity/monthly/epm_table_grapher.php?t=table_5_03.

[63] Freitas RA Jr. Economic Impact of the Personal Nanofactory. Nanotechnology Perceptions: A Review of Ultraprecision Engineering and Nanotechnology 2006 May;2:111-126; http://www.rfreitas.com/Nano/NoninflationaryPN.pdf. Freitas RA Jr. Cryostasis Revival: The Recovery of Cryonics Patients through Nanomedicine. Alcor Life Extension Foundation, 2022; Appendix G. Historical and Future Commercial Electricity Prices; https://www.alcor.org/cryostasis-revival/.

[64] Freitas RA Jr. Cell Mills: Nanofactory Manufacture of Biological Components. IMM Report No. 53, 15 June 2024; Section 2.1.2.2, Quantitative Productivity of Generic Synthesis Unit; http://www.imm.org/Reports/rep053.pdf.

[65] https://www.geoforward.com/underground-storage-tank-sizes-volumes/.

7. Implementation and Conclusions

In the scenario envisioned in this paper, all cars would likely be manufactured and sold with their 16-gallon gas tanks full of gasoline. After the automobiles enter regular use, their initial gasoline is endlessly recycled at service stations and the vehicle has zero net emissions.

If we assume N_{cars} = 200 million zero-emission gasoline-powered cars are deployed in the United States, each with a 16 gallon gas tank, then at the national level we'll be continually recycling a total of $V_{fleet} = N_{cars} V_{tank}$ = 3.2 billion gallons (~12 x 10^6 m^3) of gasoline. The 3.2 billion gallons being continually recycled is only 2.3% of the $V_{U.S.}$ ~ 136 billion gallons/yr of gasoline consumed in the U.S. in 2022.[66] When cars are retired from service, their remaining gasoline can be transferred to newly manufactured cars, eliminating the need for most petroleum extraction, transporting, and chemical processing activities for gasoline and diesel fuel production because service stations will be regenerating all replacement gasoline on site. This has environmental benefits beyond carbon emissions (e.g., fewer oil spills, etc.). An additional positive outcome is the elimination of tailpipe pollution in cities (e.g., CO, NO_x, and other smog-forming compounds), improving air quality. If successful, this scheme would drastically cut net CO_2 emissions from transport without requiring a move away from gasoline cars.

Assuming we establish $N_{stations}$ ~ 100,000 zero-emission gasoline service stations in the U.S.,[67] and assuming each car needs a complete 16-gallon refill every t_{refill} ~ 10 days, then each filling station services $N_{service} = N_{cars} / t_{refill} N_{stations}$ ~ 200 cars/day and requires a power supply of $P_{station} = (N_{service} E_{fillup} / t_{day}) + (P_{rotorsH2O} + P_{rotorsCO+UHC} + P_{rotorsNOx})$ = **10.1 MW per service station**,[68] or P_{add} = **1.01 TW** of electrical power nationwide for all 100,000 service stations in the United States, taking t_{day} = 86,400 sec/day which assumes AI-capable self-driving cars[69] can efficiently queue up to refill themselves anytime during a 24-hour day. The time required to service each car is $t_{service} \sim N_{service}^{-1}$ = 0.005 days/car = 432 sec/car ~ 7.2 min/car. The U.S. had ~**1.25 TW** of

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[66] https://www.eia.gov/energyexplained/gasoline/use-of-gasoline.php. These numbers are consistent with an average mean time between refills of (365 days/yr) (3.2 billion gallons/car) / (136 billion gallons/yr) ~ 8.6 days/car.

[67] This is about half of the 196,643 U.S. gas stations of record in 2024: Abdullah Rafaqat, "Gas Stations in United States of America," 13 Mar 2024; https://www.xmap.ai/blog/gas-stations-in-united-states-of-america-everything-you-need-to-know.

[68] If necessary, the power requirement per station can be reduced by increasing the total number of stations and correspondingly reducing the capacity of each station, while servicing the same total number of cars on the same repeat schedule. Today's big box stores such as Costco, Walmart Supercenters, or Home Depot outlets, and electric vehicle charging stations* (fast charging hubs), can draw up to 1-2 MW. In 2024 the Megawatt Charging System† was under development as a charging connector for large battery electric vehicles with a maximum power rating of 3.75 MW.
* https://en.wikipedia.org/wiki/Charging_station.
† https://en.wikipedia.org/wiki/Megawatt_Charging_System.

[69] https://en.wikipedia.org/wiki/Self-driving_car.

installed electric generating capacity in 2024,[70] so to implement the scenario envisioned here the country would need to increase its current electric generation and distribution capacity by less than double, or +81%.

In addition to the $V_{U.S.}$ ($E_{gasoline}$ / V_{tank}) / t_{year} = 0.57 TW of combustion waste heat generated by gasoline-burning vehicles as they travel, the energy cost of gasoline synthesis (Section 6.2) represents a new source of waste heat that will be released into the environment from the service stations during the octane regeneration process, in the amount of $P_{waste} = E_{octane,net}\ V_{fleet} / V_{tank}\ t_{refill}\ t_{day} \sim 0.97$ TW nationwide. This new source of waste heat is somewhat offset by the elimination of the bulk of the traditional gasoline production industry, since petroleum extraction from the ground and its subsequent refining into gasoline by traditional methods of bulk chemistry would no longer be needed, reducing waste heat production by $P_{nogasoline} \sim 0.10$ TW.[71] The net injection of $P_{heat} = P_{waste} - P_{nogasoline} \sim 0.87$ TW would increase waste heat (on top of current levels) by a relatively modest $P_{heat} / P_{consume} \sim 28\%$ over the total U.S. primary energy consumption of $P_{consume} = 3.14$ TW (93.59 quadrillion BTU) in 2024,[72] or just $P_{heat} / (P_{consume} + P_{add}) \sim 21\%$ after the U.S. adds the required 1.01 TW of new electrical generating capacity nationwide.

Handling 1000 atm gases and high-power systems at a public fuel station would require robust safety engineering, but with future materials and automation this seems manageable.

This concept illustrates how molecular manufacturing might enable a sustainable transportation loop, reusing fossil fuel carbon indefinitely. The tradeoffs – notably a larger electric grid and advanced infrastructure – are significant but within the realm of possibility given anticipated technological advances.

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[70] https://www.foley.com/insights/publications/2024/09/the-evolving-mix-of-the-energy-sources-for-the-u-s-s-electric-generating-capacity/.

[71] A crude estimate of the power consumed by the entire gasoline production chain in the U.S. might include (1) exploration for new oil deposits (1-2 GW) + (2) testing and proving out new deposits (1-2 GW) + (3) installing and operating extraction equipment at all new and existing U.S. oilfields (28-50 GW) + (4) transporting extracted crude petroleum to refineries (7-15 GW) + (5) operating the refineries to produce gasoline and related transportation-related hydrocarbon fuels (14-30 GW) + (6) transporting and distributing these fuels to end users (4-10 GW) ~ 100 GW (range 55-109 GW).

[72] https://www.eia.gov/energyexplained/us-energy-facts/.