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# Complexing $CO_2$ with a host gas before emission may delay or abrogate global warming.

Mayari G[1], Saravanakumar B[2], Apte S[3]

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**Abstract**
We evaluated the mitigation of global warming from an entirely new perspective. Assuming that $CO_2$ emissions constitute the bulk of the global warming phenomenon, we asked if irreversible complexation of $CO_2$ with another gas before emission would shift and/or abrogate its $\lambda_{max}$ from/at 15 µm and/or decrease its diffusion coefficient or effective translational velocity enough so as to decrease its absorption of Outbound Long wave Radiation (OLR) or decrease the collision rate with OLR photons respectively. We replicated the Planck's law derived spectrum of the Earth's thermal blackbody OLR log-normal curve and conservatively calculated the $CO_2$-complex contributed decrease in Earth originated spectral irradiance at 13 µm and 17 µm; when compared with that at 15 µm. We also simulated, quantified and investigated the decrease in the $CO_2$-complex diffusion coefficient by coding and running a 'Space Invaders' type video game; reminiscent of its analogous namesake in the 70s'. In both instances, there was a decrease in the amount of re-radiated radiation back to earth. In the case of the complexation mechanism, a conservative shift of ± 2 µm, was calculated to result in a decrease of 0.4 $^{o}$C in the average global temperature. In the case of the diffusion coefficient mediated mechanism, we found that a decrease of > 2X in the $CO_2$-complex diffusion coefficient – when extrapolated to a real-world speed ratio of $10^6$:1 for the OLR photons to the speed of $CO_2$ molecules - could result in a 0.2 $^{o}$C reduction in average global temperature. This decreased contribution of the diffusion mediated mechanism was exacerbated by the Graham's Law necessity of increasing the mass of the $CO_2$ molecule 4X by complexation with a permissive Lewis acid-Lewis base host gas, although our mathematically plausible calculations extrapolated at a speed ratio of $10^6$:1 were conceptually heuristic. The complexation mechanism; in contrast; did not require any minimum weight increase. Although we anticipate significant hurdles toward implementation, we believe we are the first to conceptualize this idea. If OLR absorption is reduced or abrogated by the $CO_2$-complex, there will no longer be a need to reduce (complexed) $CO_2$ emissions. The transition to greener energy sources may not be as urgent. Research is needed to find/repurpose non-toxic gases that do not contribute to greenhouse warming and which can irreversibly complex with $CO_2$, preferably under ambient conditions, so that $CO_2$ in the industrial chimney flues and automobile exhaust pipes; among others; may be mixed (and complexed) with the host gas before emission into the atmosphere.

**Keywords**
Carbon dioxide emissions, Global warming, Outgoing Longwave Radiation, Diffusion coefficient, Greenhouse gas, Carbon dioxide Capture and Storage, Anthropogenic warming, Climate change, Radiative Forcing, Environment, Decarbonization

[1]Gupil Mayari, gsm1081@g.coppellisd.com [2]Bageerathan Saravanakumar, bxs9029@g.coppellisd.com , Coppell High School, 185 W Parkway Blvd, Coppell, TX 75019, USA
[3]Corresponding author: Shireesh Apte,The Journal of High School Science. journalofhighschoolscience@gmail.com

## Introduction

Carbon dioxide ($CO_2$) capture and storage (CCS) technology is defined by the Intergovernmental Panel on Climate Change (IPCC) as "A process in which a relatively pure stream of $CO_2$ from industrial and energy-related sources is separated (captured), conditioned, compressed and transported to a storage location for long-term isolation from the atmosphere." (1). The objective of this technology is to reduce the amount of anthropogenic $CO_2$ in the atmosphere (or rather; to decrease the rate of increase of anthropogenic $CO_2$) so as to decrease (or rather; to decrease the rate of increase of) global warming. CCS is itself a complex process consisting of many steps; many of which require an input of energy; which may or may not originate from fossil fuels. The question of whether CCS is net carbon negative remains moot (2).

We deviated from this long established line of execution and instead asked these questions, "Why do we need to 'capture' this emitted $CO_2$ in the first place ? Could we not instead decrease the diffusion coefficient of this emitted atmospheric (guest) $CO_2$ (by complexing it with a host gas) so that it may collide with a lesser number of earth emitted IR radiated photons ? Could these lesser number of collisions then lead to a lesser number of $CO_2$ re-radiated photons toward the earth ? Could the complexation itself induce a shift in the $CO_2$ absorption frequency maximum of ~15 μm so that it would then absorb (and hence, subsequently re-radiate) a lesser number of Outgoing Longwave Radiation (OLR) photons? Finally, could these phenomena translate into $CO_2$ contributing to a lesser extent to the greenhouse effect ? We hypothesized that if we could irreversibly complex $CO_2$ with a heavier gas (or with a large number of light gas molecules) to reduce its diffusion coefficient; or complex the $CO_2$ gas with another gas so as to shift the former's absorption spectrum, we could – in theory – create a gaseous molecular complex weighing ~ 176 $g.mol^{-1}$ which would have an efflux rate of ~ 2X less than the parent $CO_2$ molecule; or create a marginally heavier $CO_2$-gas complex that would shift the $CO_2$ absorption spectrum enough to encounter a lesser number of OLR photons (because of the OLR spectrum peaking at 15 μm.

In the context of this work, earth re-radiated photons may be colloquially referred to as 'earth bounced photons'. This terminology is adopted to better distinguish between the re-radiated photons from the earth and the re-radiated photons from the $CO_2$ molecules. It should obviously not be taken to mean that photons somehow 'bounce' off of the earth's surface.

## Materials

The 'space invaders' simulation was coded and run on an Acer Nitro 5(AN-515-45-R6XD) with an AMD Ryzen 5 5600H CPU, Nvidia RTX 3060 Laptop GPU, and 16 GB RAM.

## Methods

Figure 1 shows the image of a captured screenshot 3.70 minutes into the simulation. The red squares represent randomly generated 'earth bounced photons', that appear at the top of the screen and make their way down with a

speed depending on the algorithm code. The black square represents a $CO_2$ molecule in the atmosphere moving at a speed – again, determined by the code – from left to right, throughout the entirety of the screen. When the coordinates of a red and a black square were the same (collision), the simulation ended and a new simulation (represented by another row; see Figure 2) began. The algorithm recorded the time taken for a black square to 'collide' with a red square from the beginning of a simulation. The algorithm was programmed to run simulations back-to-back almost instantaneously. Part of the representative data obtained are shown in Figure 2. The times for a minimum of 10345 simulations were averaged and their standard deviation, mode and median was calculated (see Tables 1 through 5). The average time for collision for a particular speed of the $CO_2$ molecule and a particular speed for the 'earth bounced photons' – the time to 'die' in the 'space invaders' game – was taken to be inversely proportional to the percentage of $CO_2$ molecules that collided with 'earth bounced photons'. Therefore, the larger this time interval, the lesser the number of $CO_2$ molecules that collided with the 'earth bounced photons'; consequently, the lesser the number of re-radiated photons and the lesser the contribution to the greenhouse effect from the atmospheric $CO_2$ molecules.

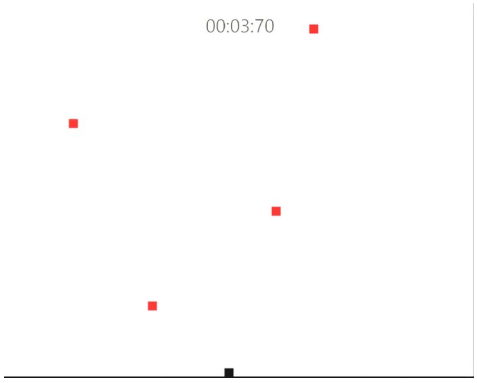


**Figure 1.** A screenshot of the simulation. The red squares represent positionally randomly generated 'earth bounced photons' which are generated at the top of the screen and move vertically downward. The black square represents a $CO_2$ molecule that moves with a velocity determined by the algorithm code from one side of the screen to another in a horizontal path. A collision of the black square with the red square ends the simulation with the time between the start of the simulation and the collision recorded by the algorithm. A subsequent simulation starts instantaneously.

The objective of the data presented in Table 1 (see later) was to show that the horizontal distance traversed by the black square (the $CO_2$ molecule) would not have an effect on the time to collision. To that end, the simulation was run only using the left or right quarters of the screen, i.e. the $CO_2$ molecule traveled one quarter of the distance horizontally, or one half of the screen (left or right). Finally, the simulation was run using the distance of the entire screen.

Graham's law of effusion, as defined by the equation, $\frac{r_2}{r_1} = \frac{\sqrt{M_1}}{\sqrt{M_2}}$, where $r_1$ and $r_2$ are the rates of effusion of gases 1 and 2 respectively and $M_1$ and $M_2$ are the molar masses of gases 1 and 2 respectively, was used to calculate the molar mass of the complexing gas as well as the molar masses of the complexed $CO_2$-complexing gas adduct so as to result in a 2X and 3X decrease in the effusion rate (approximated as the diffusion coefficient) of $CO_2$. It was calculated that a 2X reduction in the effusion rate (from setting 6 to setting 3 in the code (Appendix 1)), would require a gas molecule of molar mass 132 $g.mol^{-1}$ to complex with the $CO_2$ molecule (molar mass 44 $g.mol^{-1}$). Similarly, a 3X reduction in the effusion rate (from setting 9 to setting 3 in the code (Appendix 1)), would require a gas molecule of molar mass 1144 $g.mol^{-1}$ to complex with the $CO_2$ molecule.

| Opp Slow | Opp Mid | Opp Fast | | | Opp Slow | Opp Mid | Opp Fast |
|---|---|---|---|---|---|---|---|
| 2.21 | 2.26 | 25.63 | | **Mean** | 5.52 | 6.67 | 7.2 |
| 2.66 | 13.46 | 1 | | **STDEV** | 3.15 | 5.24 | 6.25 |
| 2.96 | 25.26 | 2.03 | | **Median** | 4.54 | 5.06 | 5.47 |
| 2.49 | 24.89 | 3.55 | | **Mode** | 2.53 | 2.02 | 1.01 |
| 4.04 | 9.11 | 4.3 | | | | | |
| 5.51 | 5.53 | 3.51 | | | | | |
| 4.64 | 7.24 | 6.54 | | | | | |
| 11.59 | 11.73 | 15.68 | | | | | |
| 3.37 | 6.46 | 15.17 | | | | | |
| 7.06 | 13.72 | 5.79 | | | | | |
| 5.02 | 2.12 | 9.09 | | | | | |
| 7.53 | 3.56 | 7.61 | | | | | |
| 2.44 | 3.04 | 1.01 | | | | | |
| 8.13 | 3.5 | 11.67 | | | | | |
| 12.67 | 2.11 | 6.08 | | | | | |
| 10.11 | 3.91 | 10.08 | | | | | |
| 3.36 | 1.54 | 18.67 | | | | | |
| 3.01 | 7.61 | 5.59 | | | | | |
| 8.58 | 4.47 | 0.97 | | | | | |
| 6.05 | 6.09 | 17.68 | | | | | |
| 3.51 | 7.8 | 3.01 | | | | | |
| 2.53 | 6.18 | 11.63 | | | | | |
| 2.52 | 14.25 | 4.03 | | | | | |
| 6 | 3.52 | 1.03 | | | | | |
| 10.03 | 3.61 | 6.57 | | | | | |
| 7.13 | 12.01 | 12.1 | | | | | |
| 8.08 | 2.99 | 19.72 | | | | | |
| 5.6 | 1.55 | 2.54 | | | | | |
| 5.51 | 4.06 | 3.55 | | | | | |

**Figure 2.** The first 30 rows/simulations (of a minimum of 10345 rows/simulations) presented in Table 4. The "Opp slow", "Opp mid" and "Opp Fast" represent the magnitude of the speed of the red squares. In all the three scenarios (3 columns), the speed of the $CO_2$ molecule was set to "Fast". The numbers in the rows represent the time in seconds taken for a red square to collide with the black square.

The earth's OLR radiation spectrum (Figure 3) was obtained from the Wikimedia web page https://commons.wikimedia.org/wiki/File:Sun-Earth_Logarithmic_Spectrums_with_Accurate_Scaling.svg . The log-normal distribution was calculated using the Open Office Calc software version 7.3.7.2 using the probability function distribution equation at https://en.wikipedia.org/wiki/Log-normal_distribution . The location parameter μ was set at 2.93 and the scale parameter of the distribution, σ, was set at 0.47 to accurately superimpose the calculated curve on that presented at Wikimedia – which itself is calculated based on the Planck's Law of Blackbody radiation at 288 K.

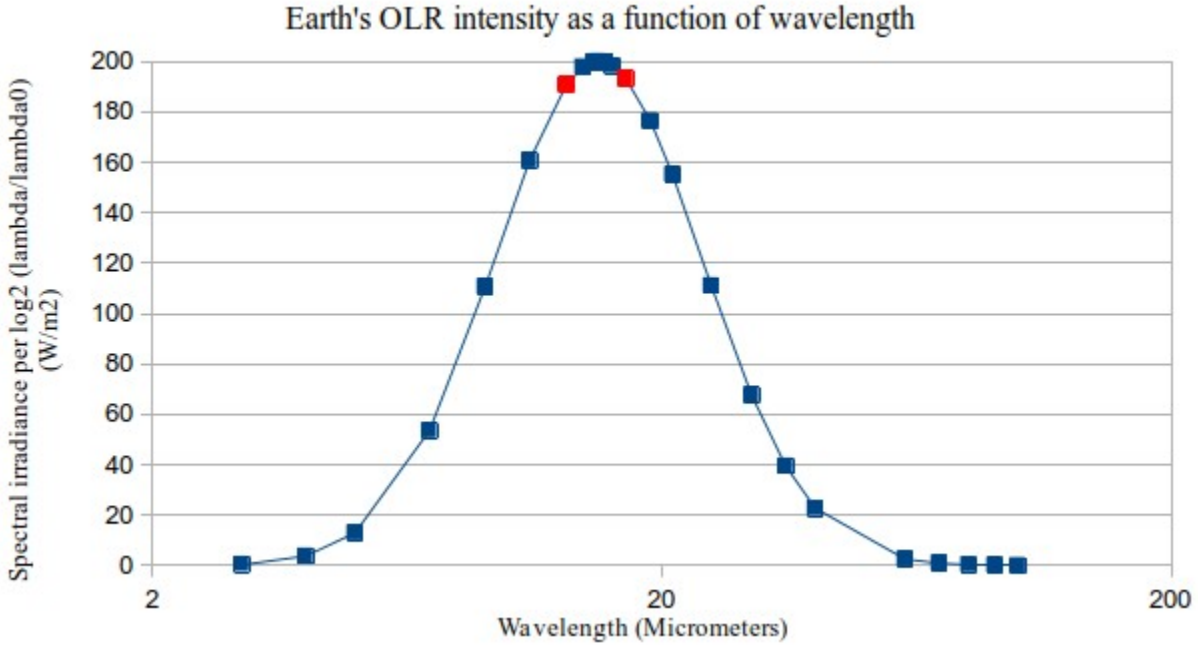


**Figure 3.** The earth's OLR -wavelength distribution. The log – normal distribution was constructed to be congruent on https://commons.wikimedia.org/wiki/File:Sun-Earth_Logarithmic_Spectrums_with_Accurate_Scaling.svg with μ = 2.93 and σ = 0.47, where μ is the location parameter and σ is the scale parameter of the distribution. The excel sheet for the exact function can be found at the GitHub repository. The red squares represent wavelengths of 13 μm and 17 μm, where the $CO_2$-permissive gas adduct is expected to absorb (shifted from 15 μm, which represents the $\lambda_{max}$ for the non-complexed $CO_2$ gas).

We used the numbers 398 $W.m^{-2}$ as the outgoing longwave radiation (OLR) emitted by the earth's surface and 239 $W.m^{-2}$ of this OLR reaching space (3-5). The greenhouse effect was hence calculated to be equivalent to [398-239] = 159 $W.m^{-2}$. 20% of this greenhouse effect (31.8 $W.m^{-2}$) was attributed to $CO_2$ (6). To calculate an approximation of the temperature decrease contributed by this complexation of $CO_2$ molecules, the net OLR reaching space before and after $CO_2$ complexation was substituted into the Stefan-Boltzmann equation, $P=\sigma T^4$, where P is the emitted energy in $J.m^{-2}.s^{-1}$, σ is the Stefan-Boltzmann constant = 5.67 x $10^{-8}$ $W.m^{-2}.K^{-4}$ and T is the absolute temperature in Kelvin.

*Statistical analysis*

p values of < 0.01 were considered significant. p values were calculated using https://www.medcalc.org/calc/comparison_of_means.php and a minimum of 10345 simulation runs for each category (speed of $CO_2$ and speed of 'earth bounced photons')

## Results

*Effect of changing the diffusion coefficient of the $CO_2$ molecule*

Tables 1 through 4 show the results of the simulation when the speed of the earth bounced photons was set equal to the speed of the $CO_2$ molecules undergoing random motion in the atmosphere. In other words, the ratio of the speeds of the earth bounced photons to the speed of the $CO_2$ molecules was 1:1. This speed ratio was then increased to $10^3$:1 for the data and analysis of Table 5. The speed ratio in actual real-world situation is expected to be $10^6$:1. More explanation regarding these ratios appears later in the manuscript.

**Table 1.** Investigating the effect of simulation start and area on collision time. The Opp was set to fast and the speed of the $CO_2$ molecule was set to 'slow'. Opp spawn interval was 500 ms.

| | Left Quarter | Left Half | Right Quarter | Right Half | Full Screen |
|---|---|---|---|---|---|
| **Mean** | 10.70 | 10.76 | 7.75 | 7.68 | 10.75 |
| **STDEV** | 6.81 | 6.91 | 6.52 | 6.37 | 6.71 |
| **Median** | 8.80 | 8.79 | 5.60 | 5.60 | 8.82 |
| **Mode** | 5.71 | 5.18 | 1.52 | 1.52 | 5.18 |

Table 1 shows that there was no effect on the horizontal distance traversed by the black square (the $CO_2$ molecule) when the simulation was run over the left quarter, left half or over the full screen. However, there was a significant decrease in mean time to collision, when the simulation was run over the right quarter or the right half of the screen. The authors cannot explain this phenomenon but speculate that it may be because; in these scenarios; the start coordinates of the black square are always set to the right bottom. Consequently, the simulations were always run full screen and the black square start coordinates were always set to the left bottom of the screen to nullify the effect of start configuration on the results. Running the simulations in this way provided evidence that the difference in the time to collide was not due to simulation set up or simulation run artifact(s).

**Table 2.** Time to collision in seconds when speed of $CO_2$ molecule was set to slow (three times slower) for three Opp speeds. Opp spawn interval was 500 ms.

| | Opp Slow | Opp Mid | Opp Fast |
|---|---|---|---|
| **Mean** | 8.52 | 10.02 | 10.17 |
| **STDEV** | 6.21 | 8.64 | 9.20 |
| **Median** | 6.58 | 7.56 | 7.56 |
| **Mode** | 3.04 | 1.52 | 1.01 |

Table 2 shows the time to collision simulated at a slow $CO_2$ molecular speed. The 'Opp' speeds effectively represent the speed of earth re-radiated IR photons. Even though photon speed is constant at 3 x $10^8$ $m.s^{-1}$, it was decided to vary it in the simulation to compare results. Unexpectedly, the 'Opp slow'- $CO_2$ slow combination resulted in the fastest time to collision among the three combinations, while the 'Opp fast' - $CO_2$ slow combination resulted in the slowest time to collision among the three combinations. This suggested that the relative speed of the two colliding entities (photon and $CO_2$ molecule) also may affect collision times, in addition to the absolute speed of the $CO_2$ molecule; which was surprising considering there was orders of magnitude of difference between their speeds: the $CO_2$ moving at the speed of sound ( ~ 3 x $10^2$ $m.s^{-1}$) and the photon moving at the speed of light (3 x $10^8$ $m.s^{-1}$). Since, the 'Opp' speed would always stay constant at 3 x $10^8$ $m.s^{-1}$, 'Opp slow' and 'Opp mid' were unobtainable in real-world situations and were thus neglected from consideration of collision times for Tables 2 through 4.

**Table 3.** Time to collision in seconds when speed of $CO_2$ molecule was set to medium (two times slower) for three Opp speeds. Opp spawn interval was 500 ms.

| | Opp Slow | Opp Mid | Opp Fast |
|---|---|---|---|
| **Mean** | 11.46 | 10.75 | 10.60 |
| **STDEV** | 5.38 | 6.71 | 7.77 |
| **Median** | 11.28 | 8.82 | 8.29 |
| **Mode** | 10.88 | 5.18 | 4.67 |

Table 3 shows time to collision results which were statistically similar to those obtained in Table 2 when the $CO_2$ molecular speed was three times slower and the speed of the earth bounced photons was set to fast (Column Opp fast), $p < 0.0007$. This suggested that slowing the $CO_2$ molecule to half its normal speed would produce a similar reduction in the percentage of $CO_2$ molecules that collided with earth bounced photons.

**Table 4.** Time to collision in seconds when speed of $CO_2$ molecule was set to fast (normal speed) for three Opp speeds. Opp spawn interval was 500 ms.

| | Opp Slow | Opp Mid | Opp Fast |
|---|---|---|---|
| **Mean** | 5.52 | 6.67 | 7.21 |
| **STDEV** | 3.15 | 5.24 | 6.25 |
| **Median** | 4.54 | 5.06 | 5.47 |
| **Mode** | 2.53 | 2.02 | 1.01 |

The results that were most consequential to the reduction of the greenhouse effect was comparing the "Opp fast" column in Table 4; which represented the collision of fast moving

$CO_2$ molecules with fast-moving 'earth bounced photons'; to the "Opp fast" columns in Tables 2 and 3; which represented the collision of slow moving $CO_2$ molecules (moving three times and two times slower respectively than those $CO_2$ molecules in Table 4) with fast-moving 'earth bounced photons'. When comparing these values (last columns) from Tables 4 and 2, it can be seen that the average times for collision were 7.2 s versus 10.2 s for the former and latter respectively ($p < 0.0001$). When comparing these values (last columns) from Tables 4 and 3, it can be seen that the average times for collision were 7.2 s versus 10.6 s for the former and latter respectively ($p < 0.0001$). Assuming that the time to collision was inversely proportional to the number of $CO_2$ molecules that collided with 'earth bounced photons', this translated into a 1.4X lesser percentage of $CO_2$ molecules collisions with 'earth bounced photons' if the speed of those $CO_2$ molecules were reduced by ½ or by 2/3$^{rds}$. In other words, the percentage of $CO_2$ molecules colliding with 'earth bounced photons' was reduced from 100% to ~ 71%, if the complexed molecule containing the $CO_2$ were to possess an effective molar mass of 176 g.mol$^{-1}$ or 1254 g mol$^{-1}$ (see later). Since we were interested in the minimum increase in molar mass, it can be seen that a minimum increase in effective molar mass of 132 g.mol$^{-1}$ [176 - 44] of the emitted $CO_2$ molecules (by complexation with another gas) was sufficient to achieve a ~ 30% reduction in collisions.

The scenario presented above however did not simulate real world conditions, where the speed of earth bounced photons is ~ $10^6$ orders of magnitude greater than the speed of $CO_2$ molecules. The 'closest' that the 'Space Invaders' simulation could replicate this real world scenario was a $10^3$:1 ratio, described and analyzed in detail below.

*Increasing the velocity ratio of earth bounced photons to $CO_2$ molecules: progressing toward a realistic scenario*

Table 5 shows the results of the simulation when the speed of the earth bounced photons was set to 1000 times the speed of the $CO_2$ molecules undergoing random motion in the atmosphere. The average times for collision were 1.7 s versus 1.6 s when the speed of the $CO_2$ molecules was increased to twice the original speed ($p < 0.0001$). The average times for collision increased from 1.5 s to 1.7 s when the speed of the $CO_2$ molecules was decreased to one-third the original speed ($p < 0.0001$). Again, assuming that the time to collision was inversely proportional to the number of $CO_2$ molecules that collided with 'earth bounced photons', this translated into a 1.1X lesser percentage of $CO_2$ molecules collisions with 'earth bounced photons' if the speed of those $CO_2$ molecules were reduced by ½. In other words, the percentage of $CO_2$ molecules colliding with 'earth bounced photons' was reduced from 100% to ~ 92%, if the complexed molecule containing the $CO_2$ were to possess an effective molar mass of 176 g.mol$^{-1}$. Since we were interested in the minimum increase in molar mass, it can be seen that a minimum increase in effective molar mass of 132 g.mol$^{-1}$ of the emitted $CO_2$ molecules (by complexation with another gas) was sufficient to achieve an ~ 8% reduction in collisions, when the speed of the earth bounced photons was 1000X that of the $CO_2$ molecules.

The Opp spawn interval represented the time between the spawning of the 'red squares', i.e. the earth bounced photons. To make comparisons consistent between different speed ratios of earth bounced photons to $CO_2$ molecules, the Opp spawn interval was heuristically adjusted at these different ratios so that between 4 and 5 'red squares' were visible in the simulation box at any given time, when the simulation was 'paused'.

**Table 5.** Time to collision in seconds when the ratio of Opp speed to the speed of the $CO_2$ molecule was set to 1000:1, 1000:2 and 1000:3 (relative speeds; not ratios) for columns Player Slow, Player Mid and Player Fast respectively. Opp spawn interval was 50 ms.

| | **Player Slow** | **Player Mid** | **Player Fast** |
|---|---|---|---|
| **Mean** | 1.71 | 1.57 | 1.52 |
| **STDEV** | 1.47 | 1.42 | 1.37 |
| **Median** | 1.33 | 1.16 | 1.11 |
| **Mode** | 0.11 | 0.11 | 0.45 |

The calculations above are valid for a earth bounced photons to $CO_2$ speed ratio of $10^3$:1. Our simulation was unable to process speed ratios > $10^3$:1. This was because there seemed to be a speed cap for the collisions due to frame caps in JavaFX, which we identified to be ~ 205 pixels per frame. Hence, in order to achieve a speed ratio of $10^6$:1, the speed of the $CO_2$ molecule (black square) would be reduced to 0.0002 pixels per frame, which was impractical in terms of the simulation mechanics. Therefore, we resorted to extrapolating at a speed ratio of $10^6$:1. In other words, since we obtained a 30% and 8% reduction in collisions at speed ratios of $10^0$ and $10^3$ respectively, we substituted a value of 2% reduction in collisions at the real-world speed ratio of $10^6$:1 so that a log-log plot of speed-ratios on the X-axis versus the percent decrease in collisions on the Y-axis yielded a linear relationship with a regression coefficient of > 0.99. This graph is shown in Figure 4. The reason we chose a log-log graph was because the radiative forcing from $CO_2$ is ~ logarithmic in concentration (7).

From Figure 4 (numbers available in the spreadsheet in the Github repository), at the real-world speed ratio of earth-bounced photons to $CO_2$ of $10^6$:1, the extrapolated log (percent) reduction in collisions between earth bounced photons and $CO_2$ molecules was 0.3010; yielding a percent reduction of 2% [$10^{0.3010}$]. This extrapolated reduction was calculated based on obtaining a straight line using the speed ratios of $10^0$:1, $10^3$:1 (both obtained from the simulation) and $10^6$:1 (the extrapolated ratio).The $CO_2$ contribution to the greenhouse effect due to this reduction the collision with earth bounced photons was calculated as, 0.98 x 31.8 $W.m^{-2}$ = 31.2 $W.m^{-2}$. The net resulting reduction in the greenhouse effect was therefore [159 – (31.8 – 31.2)] $W.m^{-2}$ = 158.4 $W.m^{-2}$; i.e. an ~ 0.38% reduction in the re-emission of OLR due to the complexation of $CO_2$ molecules with a LB-LA permissive gas.

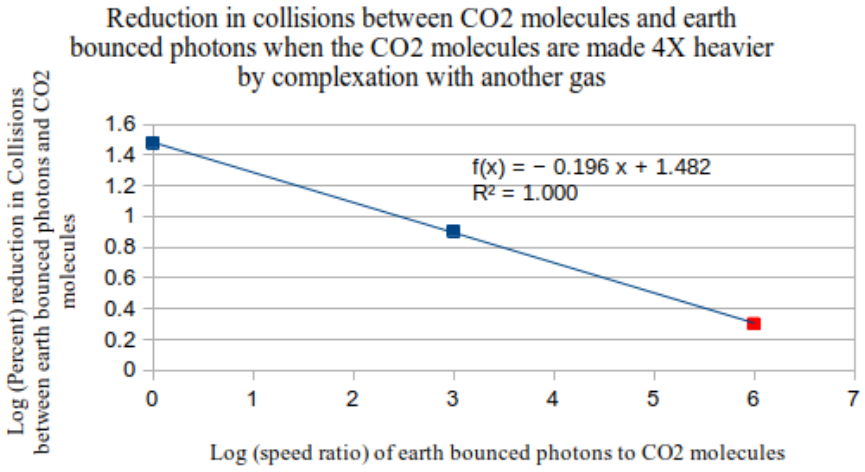


**Figure 4.** The figure shows the expected reduction in the percentage of collisions (2%, corresponding to its log of 0.3010) at a real-world speed ratio of $10^6$:1. This data point (red square on the figure) was heuristically obtained so that – when plotted with the simulation-obtained blue squares – the resultant line was linear.

To calculate an approximation of the temperature decrease that is contributed by this complexation of $CO_2$ molecules, the net OLR reaching space before and after $CO_2$ complexation of 239 $J.s^{-1}.m^{-2}$ and [239+(31.8-31.2)] = 239.6 $J.s^{-1}.m^{-2}$ respectively, was substituted into the Stefan-Boltzmann equation. Substituting the values of 239 $J.s^{-1}.m^{-2}$ and 239.6 $J.s^{-1}.m^{-2}$ into the equation for P yielded the values of 254.8 K and 255.0 K respectively for the temperatures. This implied that complexing the atmospheric $CO_2$ molecules with an LA-LB permissive gas could decrease the average temperature of the planet by (255.0 - 254.8) K = 0.20 $^oC$.

*Effect of shifting the $\lambda_{max}$ for $CO_2$ vibration by complexation with another gas*

Since the complexation of the guest $CO_2$ gas with a host gas is likely to involve Lewis-acid-base (LA-LB) type coordinate covalent bond adducts with the host gas (see later), the resultant perturbation in the stretching, bending or vibrating frequencies of the intramolecular bonds within the $CO_2$ molecule is likely to cause hypsochromic or bathochromic shifts in the absorption frequencies, depending on the relative magnitude of the LA and LB electron withdrawing or donating effects respectively (8-12). Physical adsorption of $CO_2$ causes average shifts of ~15 $cm^{-1}$, or 0.3 μm. The formation of adducts is likely to form formate, carbonate, carbamate, carboxyaldehyde, carboxylate, and formylhydroborate species; among others (13). The reaction stoichiometry and the extent of the charge separation will dictate the decrease in the absorption of the 15 μm wavelength with the concomitant emergence of other $\lambda_{max}$. As a first approximation, we used the Badger-Bauer rule, proposed by its namesake authors in 1937. They proposed that the -OH stretch frequency upon formation of H bond linearly correlates with its enthalpy change. We used a

conservative value of a frequency shift of ~ 100 $cm^{-1}$, corresponding to 40 $kJ.mol^{-1}$ (14); even though $CO_2$ adducts with permissive gases (such as with Lewis acids or Lewis bases or with frustrated Lewis pairs (15)) would most likely involve coordinate-covalent bonds with enthalpy changes of > 140 $kJ.mol^{-1}$. A shift of 100 $cm^{-1}$ corresponds to a range of ± 2 μm from a λmax = 15 μm. The spectral intensity of thermal radiation emitted by the Earth's surface follows a Log-normal distribution; the Outgoing Longwave Radiation (OLR), peaks at 15 μm, with 99% of wavelengths between 4 μm and 100 μm (16).

A linear relationship was assumed between OLR and $CO_2$-photon collisions. From Figure 3 (numbers available in the spreadsheet in the Github repository), the average spectral irradiance at 13 μm and 17 μm (the two red squares) was 96% of that at 15 μm. The $CO_2$ contribution to the greenhouse effect due to this reduction in spectral irradiance – itself a result of the shift in the $CO_2$ $\lambda_{max}$ upon complexation - was calculated as, 0.96 x 31.8 $W.m^{-2}$ = 30.5 $W.m^{-2}$. The net resulting reduction in the greenhouse effect was therefore [159 – (31.8 - 30.5)] $W.m^{-2}$ = 157.7 $W.m^{-2}$; i.e. an ~ 0.82% reduction in the re-emission of OLR due to the complexation of $CO_2$ molecules with a LB-LA permissive gas.

To calculate an approximation of the temperature decrease that is contributed by this complexation of $CO_2$ molecules, the net OLR reaching space before and after $CO_2$ complexation of 239 $J.s^{-1}.m^{-2}$ and [239+(31.8-30.5)] = 240.3 $J.s^{-1}.m^{-2}$ respectively, was substituted into the Stefan-Boltzmann equation. Substituting the values of 239 $J.s^{-1}.m^{-2}$ and 240.3 $J.s^{-1}.m^{-2}$ into the equation for P yielded the values of 254.8 K and 255.1 K respectively for the temperatures. This implied that complexing the atmospheric $CO_2$ molecules with an LA-LB permissive gas could decrease the average temperature of the planet by (255.1 - 254.8) K = 0.35 °C.

The combined decrease in global average temperature; with the caveat that the complexing gas need have a minimum molar mass of 132 $g.mol^{-1}$ was hence calculated to be 0.6 °C (0.2+0.35). The decrease in global average temperature; with no constraints on the molar mass of the complexing gas was calculated to be 0.4 °C.

**Discussion**

Several organic chemistry platforms exist to capture $CO_2$; among them are the N-heterocyclic carbenes (17), N-heterocyclic carbene-borylene complexes (18), amines (19,20), copolymerization (21,22), donor-acceptor activation (23,24). These methods either physically adsorb $CO_2$ on/in solid or liquid phases, or form Lewis-acid-base (LA-LB) type coordinate covalent bond adducts with $CO_2$ (see Figure 1 in reference 21). The LA-LB type complexes seem promising; indeed complexes of $CO_2$ with various small gaseous electrophiles or nucleophiles have been investigated with ΔG of -9 $kJ.mol^{-1}$ (25); as have complexes of dihalogenated ethyne and $CO_2$, with ΔG of up to -7.5 $kJ.mol^{-1}$ (24). The challenge is that these interactions may not be irreversible and LA-LB formation may require reaction conditions that may be onerous.

Ethylene has a molar mass of 62 $g.mol^{-1}$ and has been shown to weakly complex with $CO_2$ molecules with interaction energies of ~ -9.0 $KJ.mol^{-1}$ (26). A purely theoretical complex of Ethylene:$CO_2$ with a 2:1 molar stoichiometry would result in the complexed molecule having a mass of 168 $g.mol^{-1}$; within ± 5% of the minimum mass needed [(132+44) = 176 $g.mol^{-1}$] to achieve a 2% decrease in collision rate. However, ethylene itself is a greenhouse gas and hence does not satisfy one of the two conditions required for a complexing gas (see below). Dichlordifluoromethane (Freon-12) has a molar mass of 121 $g.mol^{-1}$. The heaviest gas is Tungston hexafluoride with a molar mass of 298 $g.mol^{-1}$, ~11 times heavier than air. It should be noted that the complexing stoichiometry need not be unimolecular. In other words, there could be > 1 molecule of gas complexing 1 molecule of $CO_2$, or the molar ratio of complexing gas to $CO_2$ may be > 1. This complexation configuration circumvents the need to discover or manufacture a gas with a molar mass of 1144 $g.mol^{-1}$. In this scenario, it may be envisaged that ~ 10 molecules of a Freon-12 like molecule may complex one $CO_2$ molecule, such that the complex may still retain the physical properties of a gas with a (complexed) molar mass of 1254 $g.mol^{-1}$. The heavier complexes may be envisaged to gradually diffuse down to earth and resultant surface concentrations may prove toxic. This conundrum hence underscores the necessity of the mass of the complexed $CO_2$ gas to not be significantly greater (than 44 $g.mol^{-1}$) so that the brownian motion supersedes sedimentation. In this context, it may be assumed that a 176 $g.mol^{-1}$ complex, would need to possess a molar volume of 1.43 x $10^5$ $cm^3.mol^{-1}$ in order to be lighter than air (density = 1.23 x $10^{-3}$ $g.cm^{-3}$). Such a large molar volume is probably not achievable, even if the atoms of the complexing gas were to be limited to consist of Fluorine, Oxygen, Nitrogen and Chlorine, since they provide the greatest electronegativity in conjunction with the smallest molar mass.

The heaviest gas is Tungsten hexafluoride with a mass of 298 $g.mol^{-1}$ and a density of 13 $kg.m^{-3}$, 1.34 times heavier than the heaviest noble gas, Radon. A gas molecule weighing 1254 $g.mol^{-1}$ must be capable of existing as a gas; even if composed of a conglomeration of lighter gas molecules. This may not seem to be a problem a'priori since the predominant requirement to exist in a gas phase is a molar density that is less than (say) 13 $Kg.m^{-3}$ – the density of Tungsten hexafluoride gas. This means that the complex will eventually diffuse to the earth's surface, unless the molar volume is large in relation to its weight (which seems improbable; see above). The complexing gas must also be non-toxic and not itself contribute to the greenhouse effect.

There exist calculations in the public domain that estimate that (at 380 ppm), there already are 40000 times the required number of $CO_2$ molecules necessary to capture all the 'greenhouse' causing IR photons (350 $W.m^{-2}$) leaving the surface of the earth. This implies that the number of $CO_2$ molecules in the atmosphere far outnumber the earth bounced photons with the energy capable of causing absorption. This is used as an argument to show that further atmospheric $CO_2$ concentration increases cannot cause an increase in global warming. However, the

calculations seem to be incorrect because they assume that all the $CO_2$ in the atmosphere is concentrated in a 1 $m^2$ cylindrical band extending from the earth's surface to ~ 12 Km (27). First approximation calculations also show that de-excitation by collision (with $N_2$ and $O_2$) molecules vastly outnumbers the re-radiation of absorbed - earth bounced photons - in the IR spectrum (28). However, this microscale approximation does not agree with macroscale observations (3-5).

Constituting 0.0417% (400 ppm) (29) of the content of the atmosphere; which weighs 5.15 x $10^{18}$ g (30), there are 2.15 x $10^{15}$ g of $CO_2$, equivalent to 4.88 x $10^{13}$ moles of $CO_2$; consisting of 2.94 x $10^{37}$ molecules of $CO_2$. Using the surface area of the earth as 510 x $10^{14}$ $m^2$ (31), there are 5.76 x $10^{20}$ molecules of $CO_2$ per $m^2$ extending to ~12 Km above the earth. Using the numbers 398 $W.m^{-2}$ as the outgoing longwave radiation (OLR) emitted by the earth's surface and 239 $W.m^{-2}$ of this OLR reaching space, the greenhouse effect is equivalent to 159 $W.m^{-2}$ (3-5). 20% of this greenhouse effect (31.8 $W.m^{-2}$) can be attributed to $CO_2$ (6). Using the energy of a 15 μm wavelength absorbing $CO_2$ photon (32) as 1.34 x $10^{-20}$ Joules, this equates to 2.37 x $10^{21}$ photon collisions per $m^2$ per s. Assuming that all these photons collide with $CO_2$ molecules, this implies 4.1 photons colliding with one $CO_2$ molecule per s. Notwithstanding the many sources of error in this back-of-the-envelope calculation, it is nevertheless instructive enough to justify the (first approximation) deployment of the 'space invaders' simulation to act as an appropriate model in order to calculate the number of photonic collisions that can be reduced with atmospheric $CO_2$ molecules by decreasing the speed (diffusion coefficient) of those molecules.

The 'earth bounced photons' collide with 8% less $CO_2$ molecules when the speed of the $CO_2$ molecules is reduced to less than ½ their original speed (at a 1:1 speed ratio). Using the calculation above, this translates into $0.92\,x\,\frac{2.37\,x10^{21}}{5.76\,x10^{20}}$= 3.79 photons colliding with one $CO_2$ molecule per s. Assuming a linear relationship between OLR and $CO_2$-photon collisions, the $CO_2$ contribution to the greenhouse effect due to the speed (diffusion coefficient) reduction can be calculated as $\frac{3.79\,x\,31.8\,W\,m^{-2}}{4.1}$= 29.36 $W.m^{-2}$. Note that a literal logical interpretation would imply that the phenomenon is still saturated with respect to $CO_2$ collisions, since both the numbers, 4.1 and 3.79 are > 1. However, since all these calculations are first approximations, we are concerned more with the magnitude of the *reduction in the heat flux* absorbed from the OLR (assuming an unsaturated regime), rather than absolute values or ratios of photons to $CO_2$ molecules. The net resulting reduction in the greenhouse effect is therefore [159 – (31.8-29.4)] $W.m^{-2}$ = 156.6 $W.m^{-2}$; i.e. a ~ 1.5% reduction in the re-emission of OLR due to a > 2X reduction in the speed of $CO_2$ molecules.

To calculate an approximation of the temperature decrease that is contributed by this decrease in the speed of $CO_2$ molecules, the net OLR reaching space before and after $CO_2$ speed reduction of 239 $J.s^{-1}.m^{-2}$ and [239+(31.8-29.4)] = 241.4 $J.s^{-1}.m^{-2}$

respectively, can be substituted into the Stefan-Boltzmann equation. Substituting the values of 239 $J.s^{-1}.m^{-2}$ and 241.4 $J.s^{-1}.m^{-2}$ into the equation for P yields the values of 254.8 K and 255.4 K respectively for the temperatures. This means that reducing the speed of atmospheric $CO_2$ molecules by > 2X, at a speed ratio of $10^3$:1 can decrease the average temperature of the planet by (255.4 - 254.8) K = 0.6 $^oC$.

Using mathematical logic similar to calculations for a $10^3$:1 ratio, beginning with the substitution of 0.98 (a reduction of 2% in the collisions between the earth bounced photons and $CO_2$ molecules (at a $10^6$:1 speed ratio) that have been slowed down 2X from their original speeds) into the equation: $0.98\,x\,\frac{2.37\,x\,10^{21}}{5.76\,x\,10^{20}}$ for a $10^6$:1 real-world ratio, the calculations result in the net OLR reaching space after $CO_2$ speed reduction of 239.6 $J.s^{-1}.m^{-2}$, corresponding to a Stephan-Boltzmann temperature of 254.9 K. This means that reducing the speed of atmospheric $CO_2$ molecules by > 2X at a real-world speed ratio of $10^6$:1 can decrease the average temperature of the planet by (255 - 254.8) K = 0.2 $^oC$.

**Limitations**

Many of the calculations and the assumptions presented in this manuscript are first approximations. Several phenomena – such as the de-excitation of the excited $CO_2$ molecules by collision with $N_2$ or $O_2$; rather than by re-emitting IR radiation – have been (conservatively) neglected. It is the bane of environmental and atmospheric science that measurements are often inaccurate, imprecise and subject to severe local effects and variations – which may or may not manifest globally - due to the sheer enormity of the scale of the model. In addition to this macroscopic capriciousness, a microscopic phenomenon such as a diffusion coefficient (which; we have assumed to serve as a surrogate for molecular speed) can only be predicted in statistical probabilistic terms. Combined together, it becomes evident that modeling atmospheric anthropogenic $CO_2$ concentration and its effect on greenhouse warming is as much an art as a science. Despite these challenges, first approximations serve – and have served – as suitable predecessors for eventual successful prediction. Furthermore, the manuscript's thrust lies in the groundbreaking idea that emitted $CO_2$ need not be captured, phase-changed and stored, akin to nuclear waste; instead, it can be complexed with a host gas and still be emitted into the atmosphere, where its greenhouse effect can then either be reduced due to a reduction in its diffusion coefficient (speed), or be reduced or abrogated due to a complexation-induced (~ ± 2 μm) shift in its absorption spectrum away from 15 μm; thus being made incapable of vibrational excitation by 15 μm earth OLR photons. The associated calculations merely serve as proof-of-concept evidence for the feasibility of the idea.

**Conclusion**

By complexing the $CO_2$ molecule with a LA-LB permissive (or other mechanism-activating) gas before the former's emission into the atmosphere, the absorption spectrum of the resultant complexed gas can be shifted ~ ± 2 μm from the earth's OLR peak of 15 μm. The resulting decrease in OLR absorption (and re-

emission) of ~ 0.82% was calculated to decrease the average earth's temperature by ~ 0.4 $^{o}$C. On the other hand, a reduction in the diffusion coefficient of the complexed $CO_2$ may not cause a significant reduction in the earth's temperature. This was because the mass of the $CO_2$-gas complex would need to be 4X the mass of $CO_2$ for a 2X reduction in its diffusion coefficient. Furthermore, calculations from the extrapolated results of the 'space invaders' simulation showed only a 2% reduction in the collisions between the earth bounced photons and $CO_2$ molecules (at a $10^6$:1 speed ratio), which would result in a ~ 0.2 $^{o}$C reduction in average global temperature. It is thus more desirable to shift the $\lambda_{max}$ of $CO_2$ excitation than to decrease its diffusion coefficient. We calculate that doing so will reduce the contribution of $CO_2$ to the greenhouse effect by ~ 0.8%, and the global average temperature by ~ 0.4 $^{o}$C. Obviously, using this model, the greater the $\lambda_{max}$ shift of the $CO_2$-gas complex, the greater the decrease in the earth's average temperature. Also, if such a bathochromic or hypsochromic shift is of a magnitude to coincide with the regime in which water vapor absorbs, the earth re-radiated OLR will not be able to excite the complexed $CO_2$, resulting in a complete abrogation of the $CO_2$ contributory greenhouse effect.

Our suggested solution does away with the problem of capturing, phase-changing and storing $CO_2$ in its entirety. This significantly reduces the need for additional industrial builds and resource allocation. It also reduces the pressure on the fossil fuel industry to transition to 'greener' sources of energy because any complexed $CO_2$ gas emissions will not increase the earth's average temperature. As the most efficient and non-onerous method of implementation of this strategy, we anticipate a separate metered feed of the (stored compressed) complexing gas at the point of emission of $CO_2$. For example, immediately downstream of the catalytic converter in automobiles exhaust pipes or in smokestack chimneys of industrial plants. When the stoichiometry of the complexing gas to $CO_2$ is > 1, there may be engineering modifications required to direct the automotive or industrial $CO_2$ effluent into a reaction chamber to be mixed with the complexing gas under specific reaction conditions; after which the complex is allowed to escape into the atmosphere.

To our knowledge, this is the first time that this idea has been presented and articulated in peer-reviewed scientific literature. We encourage the scientific community to advance its progress. Research is needed to find/repurpose low molecular weight non-toxic gases that do not contribute to greenhouse warming and which can irreversibly complex with $CO_2$ and significantly shift its $\lambda_{max}$, preferably under ambient conditions.

**Data repository**

https://github.com/bagee123/chem_space_invaders.git

**References**

1. IPCC, 2021: Annex VII: Glossary [Matthews, J.B.R., V. Möller, R. van Diemen, J.S. Fuglestvedt, V. Masson-Delmotte, C. Méndez, S. Semenov, A. Reisinger (eds.)]. In Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Masson-Delmotte, V., P. Zhai, A. Pirani, S.L. Connors, C. Péan, S. Berger, N. Caud, Y. Chen, L. Goldfarb, M.I. Gomis, M. Huang, K. Leitzell, E. Lonnoy, J.B.R. Matthews, T.K. Maycock, T. Waterfield, O. Yelekçi, R. Yu, and B. Zhou (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, pp. 2215–2256, https://doi.org/10.1017/9781009157896.022

2. Nordahl SL, Hanes RJ, Mayfield KK, Myers C, Baker SE, Scown CD. Carbon accounting for carbon dioxide removal. One Earth, 7(9), 1494-1500, 2024. https://doi.org/10.1016/j.oneear.2024.08.012

3. Chapter 7: The Earth's Energy Budget, Climate Feedbacks, and Climate Sensitivity". Climate Change 2021: The Physical Science Basis IPCC. 2021.

4. Raval A, Ramanathan V. Observational determination of the greenhouse effect. Nature, 342, 758–761, 1989. https://doi.org/10.1038/342758a0

5. Raval, A.; Ramanathan, V. (1990). "Observational determination of the greenhouse effect". Global Climate Feedbacks: Proceedings of the Brookhaven National Laboratory Workshop: 5–16. 2023.

6. Schmidt GA, Ruedy RA, Miller RL, Lacis AA. Attribution of the present-day greenhouse effect. Journal of Geophysical Research: Atmospheres, 115(D20), 2010. https://doi.org/10.1029/2010JD014287

7. Romps DM, Seeley JT, Edman JP. Why the Forcing from Carbon Dioxide Scales as the Logarithm of Its Concentration. Journal of Climate, 35(13), 4027-4047, 2022. https://doi.org/10.1175/JCLI-D-21-0275.1

8. Ye HZ, Berkelbach TC. Adsorption and vibrational spectroscopy of CO on the surface of MgO from periodic local coupled-cluster theory. Faraday Discussions, 254, 628-640, 2024. https://doi.org/10.1039/D4FD00041B

9. Moskovits M, Hulse JE. Frequency shifts in the spectra of molecules adsorbed on metals, with emphasis on the infrared spectrum of adsorbed CO. Surface Science, 78(2), 397-418, 1978. https://doi.org/10.1016/0039-6028(78)90088-2

10. Fitzgerald SA, Schloss JM, Pierce CJ, Thompson B, Rowsell JLC, Yu K, Schmidt JR. Insights into the Anomalous Vibrational Frequency Shifts of $CO_2$ Adsorbed to Metal Sites in Microporous Frameworks. J. Phys. Chem., 119, 5293-5300, 2015. http://dx.doi.org/10.1021/jp5104356

11. Zamirri L, Pantaleone S, Uglingo P. Carbon monoxide adsorption at forsterite surfaces as models of interstellar dust grains: An unexpected bathochromic (red) shift of the CO stretching frequency. J. Chem. Phys. 150(6), 064702, 2019. https://doi.org/10.1063/1.5075632

12. Delgado MR. Structure and Stability of Gas Adsorption Complexes in Periodic Porous Solids as Studied by VTIR Spectroscopy: An Overview. Appl. Sci., 10(7a), 8589, 2020. https://doi.org/10.3390/app10238589

13. Kadota K, Horike S. Conversion of Carbon Dioxide into Molecular-based Porous Frameworks. Accounts of Chem. Res., 57(21), 3206-3216, 2024. https://doi.org/10.1021/acs.accounts.4c00519

14. Kato T, Fujii A. Experimental confirmation of the Badger-Bauer rule in the protonated methanol clusters: Weak hydrogen bond formation as a measure of terminal OH acidity in hydrogen bond networks. Phys. Chem. Chem. Phys., 25, 30188-30192, 2023. https://doi.org/10.1039/D3CP04644C

15. Momming CM, Otten E, Kehr G, Frohlich R, Grimme S, Stephan GW, Erker G. Reversible metal-free carbon dioxide binding by frustrated Lewis pairs. Angew Chem. Int. Ed. Engl., 48(36), 6643-6646, 2009. https://doi.org/10.1002/anie.200901636

16. Petty GW. A first course in atmospheric radiation (2. ed.). Madison, Wisc.: Sundog Publ., 2006, p. 68. ISBN number 978-0-9729033-1-8

17. Stiernet P, Pang B, Taton D, Yuan J. The promise of N-heterocyclic carbenes to capture and valorize carbon dioxide. Sustainable Chemistry for Climate Action, 2(4), 100018, 2023. http://dx.doi.org/10.1016/j.scca.2023.100018

18. Fan J, Koh AP, Wu CS, Su MD, So CW. Carbon dioxide capture and functionalization by bis(*N*-heterocyclic carbene)-borylene complexes. Nature Communications, 15, 3052, 2024. https://doi.org/10.1038/s41467-024-47381-7

19. Jakobsen JB, Ronne MH, Daasbjerg K, Skrydstrup T. Are amines the holy grail for facilitating $CO_2$ reduction ? Angewandte Chemie, 60(17), 9174-9179, 2021. https://doi.org/10.1002/anie.202014255

20. Murphy LJ, Robertson KN, Kemp RA, Tuononen HM, Clyburne JAC. Structurally simple complexes of $CO_2$. Chemical Communications, 51, 3942-3956, 2015. https://doi.org/10.1039/C4CC08510H

21. Coates G, Allen S, Ando T. Polymers of ethylene oxide and carbon dioxide. European Patent No. EP2285864A1, Cornell University, Ithaca, NY, 2018. https://patents.google.com/patent/EP2285864A1/en

22. Acemoglu M, Nimmerfall F, Bantle S, Stoll GH. Poly(ethylene carbonate)s, part I: Syntheses and structural effects on biodegradation. J. Controlled Release, 49(2-3), 263-276, 1997. https://doi.org/10.1016/S0168-3659(97)00097-7

23. Perez-Jimenez M, Corona H, de la Cruz-Martinez F, Campos J. Donor-Acceptor Activation of Carbon Dioxide. Chemistry A European Journal, 29(61), e202301428, 2023. https://doi.org/10.1002/chem.202301428

24. Trung NT, Trang NTT, Ngan VT, Quang DT, Nguyen MT. Complexes of carbon dioxide with dihalogenated ethylenes: structure, stability and interaction. RSC Advances, 6, 31401-31409, 2016. https://doi.org/10.1039/C6RA03558B

25. Lee HM, Youn IS, Saleh M, Lee JW, Kim KS. Interactions of $CO_2$ with various functional molecules. Phys. Chem. Chem. Phys., 17, 10925-10933, 2015. https://doi.org/10.1039/C5CP00673B

26. Bauza A, Frontera A. Theoretical study on σ- and π-hole carbon...carbon bonding interactins: implications in CFC chemistry. Phys. Chem. Phys., 18, 32155-32159, 2016. https://doi.org/10.1039/C6CP06449C

27. https://issuu.com/johna.shanahan/docs/191230_count_the_molecules

28. https://geoexpro.com/recent-advances-in-climate-change-research-part-ix-how-carbon-dioxide-emits-ir-photons/

29. https://www.globalchange.gov/indicators/atmospheric-carbon-dioxide#:~:text=Panel%201%3A%20Atmospheric%20Carbon%20Dioxide&text=the%20terrestrial

%20biosphere.-,There%20is%20an%20overall%20upward%20trend%20since%20data%20collection%20began,than%2020%25%20in%2044%20years

30. Lide, David R. Handbook of Chemistry and Physics. Boca Raton, FL: CRC, 1996: 14–17

31. https://nssdc.gsfc.nasa.gov/planetary/factsheet/earthfact.html

32. Zhong W, Haigh JD. The greenhouse effect and carbon dioxide. Weather, 68(4), 100, 2013. http://dx.doi.org/10.1002/wea.2072

**Appendix 1.** Simulation code (also found in Github repository)

```
package com.example.chem_project;

import javafx.animation.Animation;
import javafx.animation.AnimationTimer;
import javafx.animation.KeyFrame;
import javafx.animation.Timeline;
import javafx.application.Application;
import javafx.event.EventHandler;
import javafx.geometry.Insets;
import javafx.geometry.Pos;
import javafx.scene.Scene;
import javafx.scene.control.Button;
import javafx.scene.control.Label;
import javafx.scene.control.RadioButton;
import javafx.scene.control.ToggleGroup;
import javafx.scene.input.KeyCode;
import javafx.scene.input.KeyEvent;
import javafx.scene.layout.Pane;
import javafx.scene.layout.VBox;
import javafx.scene.paint.Color;
import javafx.scene.shape.Rectangle;
import javafx.stage.Stage;
import javafx.util.Duration;


import java.io.*;
import java.net.URISyntaxException;
import java.util.*;


public class game extends Application {
```

```
private Stage theStage;
private Pane parent;
private Rectangle player;
private List<Rectangle> enemies;
private boolean movingRight = true;
private Label timerLabel;
private Timeline timeline;
private int milliSecondsElapsed;
boolean shouldCreateEnemy = true;
long lastCircleTime = 0;
private List<String> dataList;


int playerSpeed = 0;
int oppSpeed = 0;


String playerSpeedSetting = "";


String oppSpeedSetting = "";


int setting = 0;
final long delay = 500_000_000;
private long lastTime = 0;


private AnimationTimer timer;


@Override
public void start(Stage stage) throws Exception {
   theStage = stage;
   settingScreen();
}


private void restartGame() throws URISyntaxException {
   if(setting == 1){
      player.setTranslateX(0);
   }else if(setting == 2) {
      player.setTranslateX(0);
   }else if(setting == 3) {
      player.setTranslateX(0);
```

```
        }else if(setting == 4) {
            player.setTranslateX(730);
        }else if(setting == 5) {
            player.setTranslateX(480);
        }


        if (Objects.equals(playerSpeedSetting, "slow")) {
            playerSpeed = 3;
        }else if (Objects.equals(playerSpeedSetting, "mid")){
            playerSpeed = 6;
        }else if (Objects.equals(playerSpeedSetting, "fast")){
            playerSpeed = 9;
        }


        if(Objects.equals(oppSpeedSetting, "slow")){
            oppSpeed = 3;
        }else if(Objects.equals(oppSpeedSetting, "mid")){
            oppSpeed = 6;
        }else if(Objects.equals(oppSpeedSetting, "fast")) {
            oppSpeed = 9;
        }

        player.setTranslateY(805);
        movingRight = true;
        milliSecondsElapsed = 0;
        timerLabel.setText("00:00:000");
        enemies.forEach(enemy -> parent.getChildren().remove(enemy));
        enemies.clear();
    }

    private void settingScreen(){
        VBox vBox = new VBox();
        vBox.setPrefWidth(800);
        vBox.setPrefHeight(800);
        Scene scene = new Scene(vBox);
        vBox.setAlignment(Pos.CENTER);
        vBox.setSpacing(5);
        ToggleGroup toggleGroup = new ToggleGroup();
        ToggleGroup playerSpeedToggle = new ToggleGroup();
        ToggleGroup oppSpeedToggle = new ToggleGroup();
        Label gameName = new Label("Chem Project");
        gameName.setStyle("-fx-font-size: 60px");
        Label settings = new Label("Settings");
```

```
        settings.setStyle("-fx-font-size: 40px");
        Label speed = new Label("Speed");
        speed.setStyle("-fx-font-size: 40px");
        RadioButton rightQuarterRadio = new RadioButton("Right Quarter Screen");
        RadioButton rightHalfRadio = new RadioButton("Right Half Screen");
        RadioButton quarterRadio = new RadioButton("Left Quarter Screen");
        RadioButton halfRadio = new RadioButton("Left Half Screen");
        RadioButton fullRadio = new RadioButton("Full Screen");

        RadioButton playerSlow = new RadioButton("Player Slow");
        RadioButton playerMid = new RadioButton("Player Mid");
        RadioButton playerFast = new RadioButton("Player Fast");

        RadioButton oppSlow = new RadioButton("Opp Slow");
        RadioButton oppMid = new RadioButton("Opp Mid");
        RadioButton oppFast = new RadioButton("Opp Fast");


        quarterRadio.setToggleGroup(toggleGroup);
        halfRadio.setToggleGroup(toggleGroup);
        fullRadio.setToggleGroup(toggleGroup);
        rightQuarterRadio.setToggleGroup(toggleGroup);
        rightHalfRadio.setToggleGroup(toggleGroup);

        playerSlow.setToggleGroup(playerSpeedToggle);
        playerMid.setToggleGroup(playerSpeedToggle);
        playerFast.setToggleGroup(playerSpeedToggle);

        oppSlow.setToggleGroup(oppSpeedToggle);
        oppMid.setToggleGroup(oppSpeedToggle);
        oppFast.setToggleGroup(oppSpeedToggle);

        quarterRadio.setPadding(new Insets(0,0,0,17));
        Button startBtn = new Button("Start Game");


        startBtn.setOnAction( e->{
           if(!(quarterRadio.isSelected() || halfRadio.isSelected() || fullRadio.isSelected() ||
rightQuarterRadio.isSelected() || rightHalfRadio.isSelected())){
              System.out.println("select a setting");
           }else if(quarterRadio.isSelected()) {
              setting = 1;
              startGame();
           }else if(halfRadio.isSelected()) {
              setting = 2;
```

```
            startGame();
        }else if(fullRadio.isSelected()) {
            setting = 3;
            startGame();
        }else if(rightQuarterRadio.isSelected()) {
            setting = 4;
            startGame();
        }else if(rightHalfRadio.isSelected()) {
            setting = 5;
            startGame();
        }


        if(playerSlow.isSelected()){
            playerSpeedSetting = "slow";
            playerSpeed = 3;
        }else if(playerMid.isSelected()){
            playerSpeedSetting = "mid";
            playerSpeed = 6;
        }else if(playerFast.isSelected()){
            playerSpeedSetting = "fast";
            playerSpeed = 9;
        }


        if(oppSlow.isSelected()){
            oppSpeedSetting = "slow";
            oppSpeed = 3;
        }else if(oppMid.isSelected()){
            oppSpeedSetting = "mid";
            oppSpeed = 6;
        }else if(oppFast.isSelected()){
            oppSpeedSetting = "fast";
            oppSpeed = 9;
        }

    });


    vBox.getChildren().addAll(gameName,settings,quarterRadio,halfRadio,
            rightQuarterRadio,rightHalfRadio,fullRadio,speed,playerSlow,playerMid,playerFast,
            oppSlow,oppMid,oppFast,startBtn);


    theStage.setScene(scene);
```

```
        theStage.show();
    }


    private void stopGame() {
        if (timeline != null) {
            timeline.stop();
        }


        if (timer != null) {
            timer.stop();
        }
        // Stop other timers if any
        // Clear game state
        milliSecondsElapsed = 0;
        player.setTranslateX(0);
        player.setTranslateY(805);
        movingRight = true;
        enemies.forEach(enemy -> parent.getChildren().remove(enemy));
        enemies.clear();
    }

    private void startGame(){
        parent = new Pane();
        player = new Rectangle(20, 20);
        enemies = new ArrayList<>();
        //dataList = new ArrayList<>();
        timerLabel = new Label("00:00:000");
        timerLabel.setStyle("-fx-font-size: 40px");


        timeline = new Timeline(new KeyFrame(Duration.seconds(.01), e -> {
            milliSecondsElapsed++;
            int minutes = (milliSecondsElapsed / 6000) % 60;
            int seconds = (milliSecondsElapsed / 100) % 60;
            int hundredths = milliSecondsElapsed % 100;
            timerLabel.setText(String.format("%02d:%02d:%02d", minutes, seconds, hundredths));
        }));


        timeline.setCycleCount(Animation.INDEFINITE);
        timeline.play();
        timer = new AnimationTimer() {
            @Override
```

```
public void handle(long l) {


    if (l - lastCircleTime > delay) {
        shouldCreateEnemy = true;
        lastCircleTime = l;
    }
    if(setting == 1){
        if (movingRight) {
            player.setTranslateX(player.getTranslateX() + playerSpeed);
            if (player.getTranslateX() >= 245) {
                player.setTranslateX(245);
                movingRight = false;
            }
        } else {
            player.setTranslateX(player.getTranslateX() - playerSpeed);
            if (player.getTranslateX() <= 0) {
                player.setTranslateX(0);
                movingRight = true;
            }
        }
    }else if(setting == 2){
        if (movingRight) {
            player.setTranslateX(player.getTranslateX() + playerSpeed);
            if (player.getTranslateX() >= 490) {
                player.setTranslateX(490);
                movingRight = false;
            }
        } else {
            player.setTranslateX(player.getTranslateX() - playerSpeed);
            if (player.getTranslateX() <= 0) {
                player.setTranslateX(0);
                movingRight = true;
            }
        }
    }else if(setting == 3){
        if (movingRight) {
            player.setTranslateX(player.getTranslateX() + playerSpeed);
            if (player.getTranslateX() >= 980) {
                player.setTranslateX(980);
                movingRight = false;
            }
        } else {
            player.setTranslateX(player.getTranslateX() - playerSpeed);
            if (player.getTranslateX() <= 0) {
```

```
            player.setTranslateX(0);
            movingRight = true;
        }
    }
}else if(setting == 4){
    if (movingRight) {
        player.setTranslateX(player.getTranslateX() + playerSpeed);
        if (player.getTranslateX() >= 980) {
            player.setTranslateX(980);
            movingRight = false;
        }
    } else {
        player.setTranslateX(player.getTranslateX() - playerSpeed);
        if (player.getTranslateX() <= 730) {
            player.setTranslateX(730);
            movingRight = true;
        }
    }
}else if(setting == 5){
    if (movingRight) {
        player.setTranslateX(player.getTranslateX() + playerSpeed);
        if (player.getTranslateX() >= 980) {
            player.setTranslateX(980);
            movingRight = false;
        }
    } else {
        player.setTranslateX(player.getTranslateX() - playerSpeed);
        if (player.getTranslateX() <= 480) {
            player.setTranslateX(480);
            movingRight = true;
        }
    }
}


// Handle falling enemies
if (shouldCreateEnemy && enemies.size() < 20) {
    // Adjust the range of random values for x-coordinate
    Rectangle enemy = new Rectangle(new Random().nextInt(1001), 0, 20, 20);
    enemy.setFill(Color.RED);
    enemy.setUserData(oppSpeed);
    enemies.add(enemy);
    parent.getChildren().add(enemy);
    shouldCreateEnemy = false;
```

```
}
try {
   Iterator<Rectangle> iterator = enemies.iterator();
   while (iterator.hasNext()) {
      Rectangle enemy = iterator.next();
      int speed = (int) enemy.getUserData(); // Get the speed for this circle
      enemy.setTranslateY(enemy.getTranslateY() + speed);


      if (enemy.getTranslateY() > 1000) {
         iterator.remove();
         parent.getChildren().remove(enemy);
      } else if (enemy.getBoundsInParent().intersects(player.getBoundsInParent())) {


        /*if (setting == 1){
           System.out.println(timerLabel.getText());
           appendToLogFile(timerLabel.getText(),FILEPATH);
           //dataList.add(timerLabel.getText());
        } else if (setting == 2) {
           System.out.println(timerLabel.getText());
           appendToLogFile(timerLabel.getText(),FILEPATH);
        } else if (setting == 3) {
           System.out.println(timerLabel.getText());
           appendToLogFile(timerLabel.getText(),FILEPATH);
        }else if (setting == 4) {
           System.out.println(timerLabel.getText());
           appendToLogFile(timerLabel.getText(),FILEPATH);
        }else if (setting == 5) {
           System.out.println(timerLabel.getText());
           appendToLogFile(timerLabel.getText(), FILEPATH);
        }


         */


         if(Objects.equals(playerSpeedSetting, "slow")){
            if(Objects.equals(oppSpeedSetting, "slow")){
               System.out.println(timerLabel.getText());
               //appendToLogFile(timerLabel.getText(), FILEPATH);
            }else if(Objects.equals(oppSpeedSetting, "mid")){
               System.out.println(timerLabel.getText());
               // appendToLogFile(timerLabel.getText(), FILEPATH );
```

```
                    }else if(Objects.equals(oppSpeedSetting, "fast")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }
                }else if(Objects.equals(playerSpeedSetting, "mid")){
                    if(Objects.equals(oppSpeedSetting, "slow")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }else if(Objects.equals(oppSpeedSetting, "mid")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }else if(Objects.equals(oppSpeedSetting, "fast")){
                        System.out.println(timerLabel.getText());
                        //appendToLogFile(timerLabel.getText(), FILEPATH );
                    }
                }else if(Objects.equals(playerSpeedSetting, "fast")){
                    if(Objects.equals(oppSpeedSetting, "slow")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }else if(Objects.equals(oppSpeedSetting, "mid")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }else if(Objects.equals(oppSpeedSetting, "fast")){
                        System.out.println(timerLabel.getText());
                        // appendToLogFile(timerLabel.getText(), FILEPATH );
                    }
                }
                restartGame();
            }
        }
    }catch (Exception ex){


    }
  }
};


timer.start();
parent.setPrefWidth(1000);
parent.setPrefHeight(1000);
parent.getChildren().add(player);
parent.getChildren().add(timerLabel);
if(setting == 1){
   player.setTranslateX(0);
```

```
    }else if(setting == 2) {
       player.setTranslateX(0);
    }else if(setting == 3) {
       player.setTranslateX(0);
    }else if(setting == 4) {
       player.setTranslateX(730);
    }else if(setting == 5) {
       player.setTranslateX(480);
    }


    if (Objects.equals(playerSpeedSetting, "slow")) {
       playerSpeed = 3;
    }else if (Objects.equals(playerSpeedSetting, "mid")){
       playerSpeed = 6;
    }else if (Objects.equals(playerSpeedSetting, "fast")){
       playerSpeed = 9;
    }


    if(Objects.equals(oppSpeedSetting, "slow")){
       oppSpeed = 3;
    }else if(Objects.equals(oppSpeedSetting, "mid")){
       oppSpeed = 6;
    }else if(Objects.equals(oppSpeedSetting, "fast")) {
       oppSpeed = 9;
    }
    player.setTranslateY(805);
    timerLabel.setTranslateX(430);
    timerLabel.setTranslateY(50);
    Scene scene = new Scene(parent);
    scene.setOnKeyPressed(new EventHandler<KeyEvent>() {
       @Override
       public void handle(KeyEvent keyEvent) {
          if (keyEvent.getCode() == KeyCode.B){
             stopGame();
             settingScreen();
          }
       }
    });
    theStage.setTitle("Chem");
    theStage.setScene(scene);
    theStage.show();
  }
  private void appendToLogFile(String message,String filename) {
```

```
      try {
         FileWriter fw = new FileWriter(filename, true);
         fw.write(message);
         fw.write("\n");
         fw.close();
      }
      catch(IOException e) {
      }
   }
   public static void main(String[] args) {
      launch();
   }
}
```