Simulating a Rocket Engine to Optimize Fuel Efficiency

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We model a simplified rocket engine to find parameters of pressure and temperature sufficient to accelerate a satellite of $1,000kg$ to escape velocity within 20 minutes. When calculating physical quantities with our model, we find good correspondence with analytical expressions, supporting its accuracy. With a somewhat realistic temperature of $4,000K$, a successful rocket requires about 66.9 tonnes of fuel. Finding ways to increase the temperature beyond this current limit could improve fuel efficiency; in our model, high temperatures allow for much lower densities, and in the extreme at $36,000K$ we need only 5.8 tonnes of fuel.

I. INTRODUCTION

Space exploration is of central interest in modern times, and the essential first step is to break free from the gravitational chains of our home planet. Any rocket launch requires enormous resources, and it is vital to develop good models with which one can tune variables such as density and temperature to save resources. We explore one such model and use it to simulate a rocket launch on a sample planet of slightly more challenging conditions than the Earth (albeit with no atmospheric drag), aiming to find a cost-effective solution.

A rocket engine works by heating gas and releasing it downwards. By Newton's third law, the accelerated exhaust leaving the rocket gives an equal reaction thrusting the rocket upwards. One simple way to model this involves simulating a small box of particles with a hole in the bottom and calculating the total momentum escaping the box in a short time step. This momentum is imparted to the rocket, and assuming constant pressure and temperature, this gives a constant thrusting force. Thus, we only have to model a short duration to find the thrust force on the rocket throughout the 20 minutes.

Beyond the assumption of constant pressure and temperature in our box, which is achieved in our model by the inflow of hot gas from the combustion chamber (Figure 1), we shall make several simplifying assumptions of varying severity.

First, we will use the ideal gas approximation, assuming no interaction between molecules and elastic collisions with the box walls. At high temperatures, the particle speeds should be sufficiently large that it is reasonable to disregard inter-molecular forces, and though our modelled box is small, the very highest gas density we will use is in the order of magnitude of 0.01 mol/L, so this assumption should be uncontroversial.

Second, we neglect the atmospheric drag of our planet. This means that one should be careful when applying our results to rockets launched on Earth. However, our simulation can be modified to include air resistance if the drag coefficient gradient of the rocket through the thinning atmosphere is known.

Third, while we launch our rocket vertically, we use the escape velocity at ground level as our goal velocity. This means that we overshoot the escape velocity and thus are not fully efficient. Compared to disregarding atmospheric drag, this is a gentle assumption.

Fourth, we ensure that the vertical speed distribution in the box is constant to ensure a constant thrust. This might not be entirely accurate, since, in reality, the particles starting with large vertical velocities quickly escape through the hole while particles with small vertical velocities will stay in the box for a long time. Still, we require constant thrust to save computation.

Finally, we dissect the engine into tiny boxes and model only one such box, containing a very small portion of the total gas. This could be problematic if the velocities of some particles become so large that they move a large fraction of the length of our box in one model time step. However, this is only a concern at ridiculous temperatures of 40,000K with the smallest box lengths of 0.1 micrometres for the very fastest particles. In this case, the particles may move nearly a third of the box length in one time step, potentially placing them well outside the box (as illustrated in Figure 2), but this is so rare that it should be of no concern. Either way, we demonstrate that the thrust obtained from our model corresponds to the analytical thrust we will derive in the next section.

We also model a very simple launch disregarding fuel weight and gravity at 10,000K with a box length of 1 micrometre and test the modelled pressure, mean speed and mean kinetic energy against the analytical values.

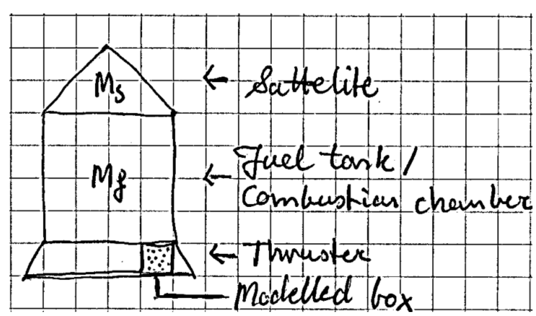

Figure 1. *Our simplified rocket as in [1]. The satellite has mass $M_s = 1000kg$. The fuel with mass M_f is stored in the rocket body. The combustion chamber above the thruster heats the fuel and pushes it to the model engine. We model only one tiny box of side length L containing $N = 100,000$ particles and multiply up to get the total thrust.*

II. THEORY

To test the accuracy of our model, we will quickly build on the expressions from [1] to derive analytical expressions for pressure, mean speed, mean kinetic energy and thrust. The ideal gas law $P = nkT$ [1], where P is the pressure, n is the number of particles per volume, k is the Boltzmann constant and T is the temperature, directly relates the pressure to the temperature of an ideal gas.

Letting m be the mass of a single H_2-molecule, we use the Maxwell-Boltzmann distribution function

$$P(v) = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}}, \quad [1]$$

to calculate the mean speed $\langle v \rangle = \int_0^\infty vP(v)dv$ by substituting $u = \frac{mv^2}{2kT}$ and using that $\int_0^\infty e^{-u}du = \Gamma(1) = 1$. This gives

$$\langle v \rangle = \sqrt{\frac{8kT}{\pi m}} \tag{1}$$

Similarily, we can calculate the mean kinetic energy $\left\langle \frac{1}{2}mv^2 \right\rangle = \frac{1}{2}m\left\langle v^2 \right\rangle = \frac{1}{2}m\int_0^\infty v^2P(v)dv$ using the same substitution and properties of the gamma-function

$$\int_0^\infty u^{\frac{3}{2}}e^{-u}du = \Gamma(\frac{5}{2}) = \frac{3}{2}\frac{1}{2}\Gamma(\frac{1}{2}) = \frac{3\sqrt{\pi}}{4}$$

to get

$$\langle E_K \rangle = \frac{3}{2}kT \tag{2}$$

Finally, we calculate the thrust F_T. Let P be the pressure, assumed to be constant and given by the ideal gas law, let A_h be the area of the hole, let F be the force on an imaginary surface covering the hole and let $\mathrm{d}p_z$ be the total change in momentum of the particles colliding elastically with this imaginary surface in a short time frame. If we denote the total change in momentum inside the box by $\mathrm{d}p_{esc}$ and the speed in the z-direction of the i-th particle as v_i one should notice that $\mathrm{d}p_z = \sum_i 2mv_i = 2\sum_i mv_i = 2\mathrm{d}p_{esc}$ (This should be evident from Figure 2). Thus,

$$nkT = P = \frac{F}{A_h} = \frac{1}{A_h}\frac{\mathrm{d}p_z}{\mathrm{d}t} = \frac{2}{A_h}\frac{\mathrm{d}p_{esc}}{\mathrm{d}t} = \frac{2F_T}{A_h},$$

and solving for the thrust we get

$$F_T = \frac{1}{2}A_h nkT \tag{3}$$

We will also need the escape velocity v_{esc} at a planet's surface, which is the smallest sufficient speed to escape its gravitational well. By equating the kinetic energy to the gravitational potential energy, with G as the gravitational constant, M_p as the planet's mass and R_p as its radius, one easily finds that

$$v_{esc} = \sqrt{\frac{2GM_p}{R}}.$$

III. METHOD

We model $N = 100,000$ particles in a box of side length L ranging from 0.1 to 1 micrometres (Figure 3), drawing the components of the particle positions from a uniform distribution [0, L) and the particle velocities from the Maxwell-Boltzmann distribution given in [1]. Our temperature T ranges from $4,000K$ to $40,000K$. The ranges on L and T take as a starting point values which are not too unrealistic, with one order of magnitude in leeway.

In simulation, we move the particles with a time step of one picosecond for a total time $\Delta t = 1ns$, keeping track of the number of escaped particles and the total momentum loss. In an ideal gas, each molecule has constant velocity until it bounces elastically against a wall, which changes the sign of the velocity component normal to the wall. We do not mirror the position through the wall, as would reflect the fully drawn line in Figure 2, using instead the approximation drawn with dotted lines, which is very good except potentially at very unrealistic conditions for some outliers in the Maxwell-Boltzmann distribution.

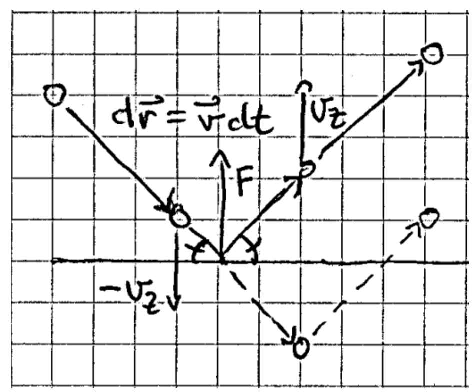

Figure 2. *A simulated particle through three time steps colliding with a plane. The change in position between consecutive time steps is* $\mathrm{d}\mathbf{r} = \mathbf{v}\mathrm{d}t$*, where* $\mathbf{v}$ *is the particle's velocity and* $\mathrm{d}t = 1ps$ *is our time step. The fully drawn line denotes the correct elastic collision with a plane, while the dotted line denotes our approximation, simply inverting the normal velocity without mirroring the position through the plane. When* $\mathrm{d}\mathbf{r}$ *is small compared to the box length* L*, this is an excellent approximation. Evidently, the change in momentum of the particle perpendicular to the plane, say the z-direction, from the elastic collision in the second time step is* $2mv_z$*, which is due to a force* F *from the plane on the particle. By Newton's third law, this entails a pressure from the gas on the plane. An escaping particle carries a momentum* $p_z = -mv_z$ *out of the rocket, increasing the rocket's momentum by the inverse amount.*

To keep the speed distribution in the box constant, one may simply let the particles bounce back (using again the dotted approximation of Figure 2), as if the box were closed, when hitting the 'hole', which is the subset of the xy-plane $\left[0, \frac{L}{2}\right) \times \left[0, \frac{L}{2}\right)$ (Figure 3). Alternatively, one could teleport the escaping particles to the top of the box without changing the velocity to simulate the inflow from the combustion chamber closer. We chose the simplest way in our simple launch disregarding gravity and fuel mass since we already made such severe approximations and the teleportation could interfere with our pressure calculations. However, in the final calculations of fuel cost as a function of temperature and box length (Figure 6), we use the slightly more complicated simulation.

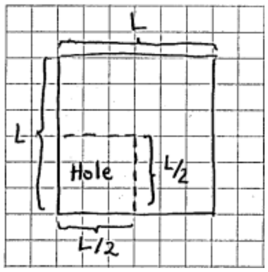

Figure 3. *The bottom plane of the modelled tiny box. The hole is drawn with dotted lines, with side length* $L_h = \frac{L}{2}$*. For simplicity, we place the hole in the bottom left corner; only the fractional area is of consequence. Notice that the total hole area is a fourth of the full thruster area.*

By conservation of momentum, we can now calculate the momentum imparted to the rocket per box per Δt, which by Newton's second law is the thrust per box. Dividing the thruster area A, which we somewhat arbitrarily set to 10 square metres, by the box area $A_b = L^2$ gives the number of boxes. Multiplying the modelled thrust per box by the number of boxes, we indeed get excellent correspondence with the theoretical thrust, which we obtain from equation (3) using $A_h = (^L/_2)^2$ and $n = {^N/_{L^3}}$, as can be seen in the results section.

The acceleration due to gravity is given by

$$a_g = -G\frac{M_p}{h^2},$$

where G is the gravitational constant, $M_p \approx 1.15 \cdot 10^{24} kg$ is the mass of our planet and h is the time dependent height from the planet centre. The starting height is the planet radius $R_p \approx 7.79Gm$. Our planet's mass is thus about 1.92 times greater than the Earth's, while the radius is about 1.22 times greater. Both the mass and the radius are retrieved from the 'home planet' of the SolarSystem class with seed 69042 in the ast2000tools python module.

The rocket acceleration a_T due to the thrust is given by dividing the total thrust force by the rocket mass M, which is time-dependent. Since we have tracked the number of escaping particles N_{esc} in a time frame Δt, we can calculate the burn rate $\alpha = \frac{mN_{esc}}{\Delta t}$. The total mass of fuel required to keep the thrusters blasting for $t_{goal} = 20min$ is then $M_f = \alpha t_{goal}$ and the rocket mass is given as a function of time by $M(t) = (M_s + M_f) - \alpha t$.

This way of calculating the starting mass, requiring enough fuel to last the entire 20 minutes, introduces an important nuance in our model. Since the force of gravity depends on the rocket mass, while the thrust is constant, it turns out that for all realistic temperatures, the most fuel-efficient rockets spend several minutes glued to the ground with a thrust lower than the surface gravitational pull. Eventually, they have wasted so much fuel mass that the thrust overcomes gravity. At these temperatures, one would need incredible gas densities to immediately overcome the gravitational pull, which would require a truly gargantuan amount of fuel (Note the difference in scale on the colourbars of figures 5 and 6), and would launch our rocket to speeds vastly exceeding the goal of escape velocity.

Another way to see this is to pin down the temperature and require instantaneous take-off by terminating all launches where the initial acceleration is negative. Then, one can vary the box length, which determines the gas density, to find the minimum required density to achieve instantaneous take-off. The speed of this rocket after 20 minutes is the *minimum required final speed* v_{req} at the given temperature. Indeed, for realistic temperatures, v_{req} is much greater than v_{esc}; so much so that it is incredibly beneficial to instead initially waste fuel and reach escape velocity in a shorter time frame (Figure 4 gives a useful illustration of this point).

Of course, one should simply subtract from M_f the wasted fuel $M_w = \alpha t_w$, where α is the burn rate and t_w is the time wasted before the thrust overcomes gravity, and start immediately with only the required amount of fuel to reach escape velocity in less than 20 minutes. These adjusted numbers are the ones we will provide because they are the values relevant in a real-world situation where one is concerned with reaching escape velocity as cheaply as possible within a given time frame. In reality, one would obviously not fill the rocket with so much fuel as to vastly overshoot escape velocity.

With this in mind, we can finally model the rocket flight. We use the Euler-Cromer method with a time step of 0.1 seconds, updating first the mass by subtracting $\mathrm{d}M = \alpha \mathrm{d}t$ and then obtaining the acceleration $a = a_t + a_g$ as described above. Note that the acceleration due to gravity a_g has a negative sign and is inversely dependent on the square of the height of the rocket; therefore, it diminishes with time when the rocket has left the ground. The acceleration due to the thrust is inversely related to the mass of the rocket and thus increases with time. Clearly, we may terminate the loop as soon as escape velocity is reached, since we have no interest in overshooting this velocity but care only to find the most efficient successful launch.

When requiring instantaneous takeoff, we terminate the loop if the initial acceleration is negative. Else, we simply set the speed to zero and continue looping, since the normal force keeps the rocket from moving through the planet surface. In light of the previous discussion, we importantly also keep track of the time until the acceleration is positive so that we can subtract the wasted fuel from the initial fuel to find the minimum required fuel.

Finally, to test our model, let us temporarily pin down $T = 10,000K$ and $L = 1\mu m$ and disregard fuel weight and gravity. Note that this is excessive to reach our goal;

we have constant mass $M = 1000kg$ giving constant acceleration and have described how to find this acceleration with our model by multiplying the modelled acceleration per box a_b by the number of boxes. Thus, the number of boxes needed to reach v_{esc} in $t_{goal} = 20min$ is

$$N_B = \lceil \frac{v_{esc}}{a_b t_{goal}} \rceil.$$

This gives an area of 6.8 square meters, accommodating about 6.8 trillion boxes, as sufficient to succeed. Indeed, a temperature of 10,000K is unrealistic, but we are already disregarding fuel weight and gravity; this is not a realistic launch, but a test of the engine model against the analytical values.

We model the pressure by tallying up the total change in z-momentum Δp_z of the particles bouncing off the bottom of the box. Then $F \approx \frac{\Delta p_z}{\Delta t}$ and $P = \frac{F}{A_b}$. Indeed, we get excellent correspondence with the equation of state. The average speed is simply calculated as $\frac{1}{N}\sum_i u_i$ where u_i is the speed of the i-th particle, and similarly the average kinetic energy is $\frac{1}{2}m \cdot \frac{1}{N}\sum_i u_i^2$. Again, we get highly similar values with the analytical formulas of equation (1) and (2), as we will see in the next section.

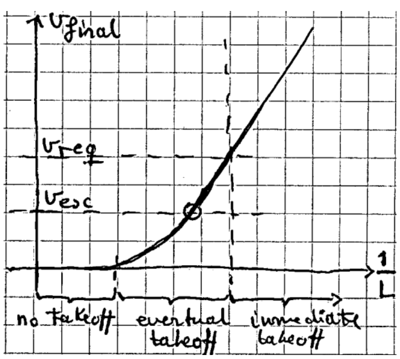

Figure 4. *An artistic rendition to illustrate the minimum required speed for a given temperature. We pin down the temperature T and graph the velocity after 20 minutes v_{final} against the inverse of the box length L. Each point on the first axis corresponds to one rocket launch: Initially, the gas density is so low that the rocket thrust never exceeds the weight of the satellite so that the rocket never takes off. At higher densities, the rocket is initially too heavy to take off and wastes fuel until it is sufficiently light to leave the ground. Notice that, for our given temperature, the rocket which reaches escape velocity after exactly 20 minutes, marked with a circle, is among these wasteful rockets. Finally, we have the rockets which take off immediately. These have ridiculous densities and burn a truly astounding amount of fuel. Importantly, the graph is* not *to scale and has a non-linear $^1/_L$-axis for compact illustration; in reality, the effect is much more drastic, as is clear from the Results section and figures 5 and 6.*

IV. RESULTS

In our test launch, we find a signed relative difference of -0.805% between the modelled pressure and the equation of state, counting just over $250,000$ collisions with the bottom plane in $\Delta t = 1ns$. The signed relative difference between mean speed and equation (1), and mean kinetic energy and equation (2), are respectively 0.12% and 0.21%. Our test launch finally gives a signed relative difference of -0.61% between the modelled thrust and equation (3) and uses 1.7 tonnes of fuel.

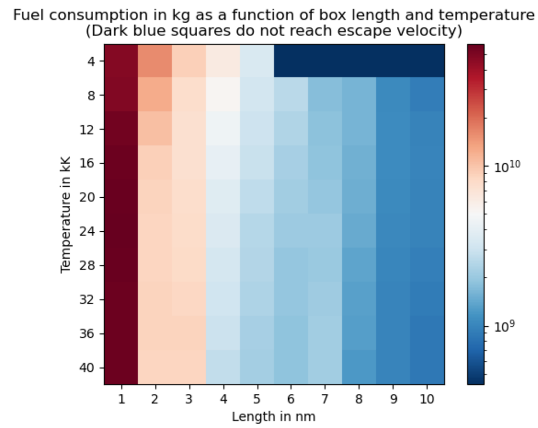

Figure 5. *Logarithmic heat map of fuel use for different temperatures and box side lengths, here requiring instantaneous takeoff. In comparison to Figure 6, note the* huge *difference in scale on the colourbars, which results from the difference in box length. Beware that at these lengths our assumptions are slightly dubious; fuel values should be read off only approximately. We refer to the method section and Figure 4 for an extensive discussion of the different approaches.*

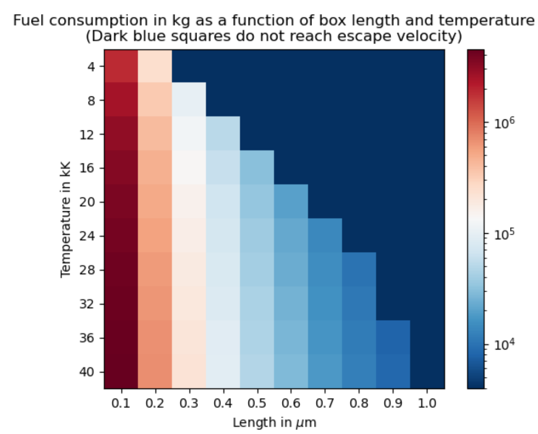

Figure 6. *Logarithmic heat map of fuel use for different temperatures and box side lengths, here optimising for fuel efficiency. Note that we include the fuel wasted on the ground. As one might expect, increasing the temperature increases the fuel cost at a given box length, but allows for lower gas densities, which turns out to have a much greater effect. Thus, one should use as high a temperature as possible and then find the lowest sufficient density (that is, the largest box length still reaching escape velocity) to maximise fuel efficiency.*

The best instantaneous takeoff at 4,000 K requires about 0.5 giga-tonnes of fuel, while the best rocket at the same temperature uses only 240.1 tonnes, including wasted fuel. This best rocket spends an astounding 14.3 minutes on the ground, wasting 172.2 tonnes of fuel to reach escape velocity in exactly 20.0 minutes. Thus, one needs only 66.9 tonnes of fuel to reach escape velocity in only 5.7 minutes with this rocket.

If we allow higher temperatures, it is clear from Figure 6 that one can dramatically improve fuel efficiency; at 36,000 K one could reach escape velocity in 14.3 minutes with only 5.8 tonnes of fuel.

[1] Hansen, F. K., 2017, Lecture note 1A for the course AST2000 at UiO.