Model Documentation

This is a very simple model to simulate the transformation of two different kinds of gas particles NO and O_3 into NO_2 and O_2 in a 2-dimensional space. The assumption is made, that the reaction is irreversible (this is not true in reality!). The process only takes place if two particles collide and their collision energy exceeds a certain threshold. The considered reaction

$$NO + O_3 \longrightarrow NO_3 + O_2$$

is exothermic. That means additional kinetic energy is added to the system. In other words, the particles speed up after reacting. In reality the mass is changing too, but this is not implemented (yet).

Velocity Distribution of Particles

The probability density function of a particle's velocity distribution in one dimension is given by

$$p(v)\mathrm{ds} = \sqrt{\frac{m}{2\pi k_B T}} e^{\frac{-mv^2}{2k_B T}} \mathrm{ds}$$

where T denotes the temperature in Kelvin, m the particle's mass in Kilogram, $|v|$ the absolute value of the velocity in meter per second and $k_B = 1,380649 \times 10^{-23} J/K$ is the Bolzmann constant. This can be applied to the the independent variables v_x and v_y where $v = (v_x, v_y)$ denotes the velocity in Cartesian coordinates. The density function can be written as

$$p(v_x, v_y)\mathrm{dxdy} = p(v_x)p(v_y)\mathrm{dxdy} = \frac{m}{2\pi k_B T} e^{\frac{-m(v_x^2+v_y^2)}{2k_B T}} \mathrm{dxdy}$$

In two dimensions the Euclidean norm of v can is $r := |v| = \sqrt{v_x^2 + v_y^2}$. We are only interested in the absolute value of the velocity. Therefore we transform the density function in polar coordinates, integrate the angle over the interval $[0, 2\pi)$ and get

$$p(v_r)\mathrm{dr} = 2\pi r \frac{m}{2\pi k_B T} e^{\frac{-mr^2}{2k_B T}} \mathrm{dr} = r \frac{m}{k_B T} e^{\frac{-mr^2}{2k_B T}} \mathrm{dr}.$$

The expected value of the absolute velocity can be calculated by

$$\mathbb{E}[v_r] = \int_0^\infty r p(v_r)\mathrm{dr} = \sqrt{\frac{\pi k_b T}{2m}}.$$

The standard deviation is given by

$$\mathrm{std}[v_r] = \sqrt{\int_0^\infty (r - \mathbb{E}[v_r])^2 p(v_r) \mathrm{d}r} = \sqrt{\frac{k_b T}{m}(1 - \frac{\pi}{4})}$$

A reaction between two particles P_1 and P_2 only happens if their relative kinetic energy E_{rel} is larger than the needed threshold energy E_0. For $i \in \{1, 2\}$ let m_i be P_i's mass and v_i is P_i's velocity. By v_c denote the velocity of the collision system's center of gravity and by $v_i \cdot n$ denote the Euclidean projection of the velocity on the normal of impact. Due to conservation of momentum the equality

$$v_1 m_1 + v_2 m_2 = v_c(m_1 + m_2) \tag{1}$$

holds. In a fully elastic collision the kinetic energy is preserved. Splitting the total kinetic energy of the collision system into the kinetic energy of the center of gravity and the relative kinetic energy results in

$$\frac{m_1 |v_1|^2}{2} + \frac{m_2 |v_2|^2}{2} = \frac{M |v_c|^2}{2} + E_{\mathrm{rel}}$$

where $|.|$ denotes the Euclidean norm and $M = m_1 + m_2$.
Defining the so called reduced mass as

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

E_{rel} can be expressed as

$$E_{\mathrm{rel}} = \frac{\mu}{2} |v_1 - v_2|^2$$

using (1) to eliminate v_c.

Simulate an Exothermic Reaction

For simplicity it is assumed, that both particles speed up by a percentage α. By This factor can be determined by solving the following equation for α

$$\alpha(E_{\mathrm{kin}_1} + E_{\mathrm{kin}_2}) = \frac{E_{\mathrm{kin}_1} + E_{\mathrm{kin}_2} + \Delta E}{E_{\mathrm{kin}_1} + E_{\mathrm{kin}_2}}$$

where $E_{\mathrm{kin}_i} = \frac{m_i v_i^2}{2}$ and ΔE denotes the energy released by the reaction. The kinetic energy has to be scaled by

$$\alpha = 1 + \frac{\Delta E}{E_{\mathrm{kin}_1} + E_{\mathrm{kin}_2}}.$$

The mass remains constant. Therefore v_1 and v_2 are multiplied by $\sqrt{\alpha}$ to get the desired output.

Parameters and Scaling

To be done. The model is not scaled at the moment. This means the parameters are fictional.