The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

First Principles Modeling of the Performance of A HYDROGEN-PEROXIDE-DRIVEN CHEM-E-CAR

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In this study, basic principles of thermodynamic, heat, and momentum transfer,[1-3] are used along with the conservations laws of mass and energy to simulate the transient conditions of a reaction-driven car or so-called "Chem-E-Car." Chem-E-Car competitions are held in countries around the world to improve teamwork skills of university students in addition to providing them with a practical situation for applying their theoretical knowledge. Chem-E-Car is a shoe-box-size car that should be able to carry a specific load within a given range (*i.e.*, 0 to 500 g) up to a precise distance within a given range (*i.e.*, 15 to 30 m).[4] Typically, these ranges are given to competitors a few months in advance, but the specific values of load and distance will be announced on the competition day. The closest car to the destination line will be the winner. Teams are free to use any chemical reaction to drive the car but they are not allowed to employ any mechanical brake to stop the car at the desirable point. Therefore, the car should be supplied with an accurate amount of fuel to stop as closely as possible to the final destination line. The most popular Chem-E-Car engines are based on the production of a pressurized gas by decomposition of a substance or by a reaction of an acid or base with a neutral salt. Also, combustion of hydrocarbons and fuel cells are considered as other alternative methods. Several trial runs should be performed prior to the competition to identify the behavior of the constructed car. Simulation of the system has some great advantages both in the design stage and for decision making on the competition day. In the design phase, the model can be used to obtain the

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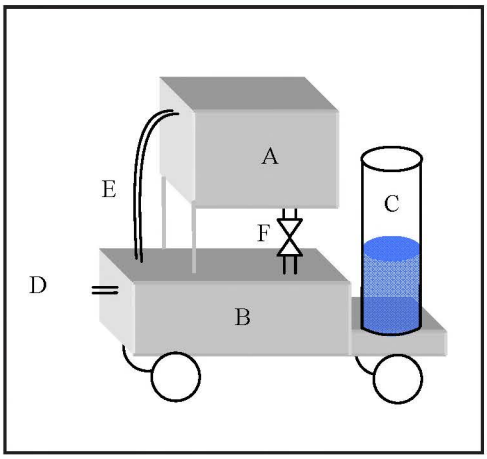

Figure 1. *Schematic of the proposed car: fuel tank (A), reaction chamber (B), external load vessel (C), exit nozzle (D), connecting hose (E), and fuel valve (F).*

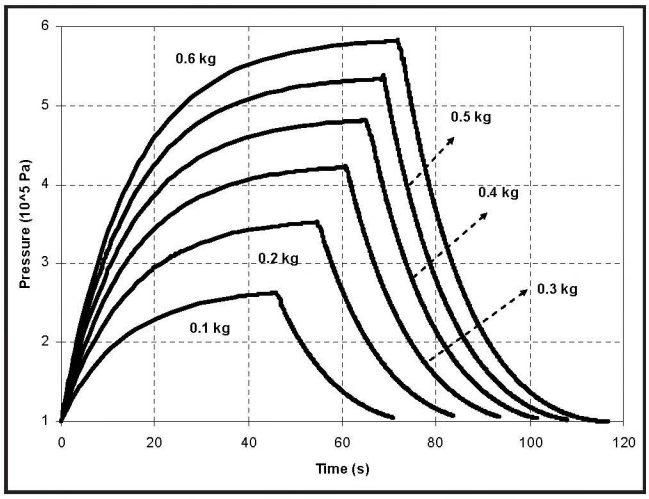

Figure 2. *Absolute pressure vs. time for different initial fuel weights.*

maximum expected pressure, thus, the machine's vessel can be constructed with a proper thickness. More importantly, sensitivity analyses of the different potential engines and vessel sizes would help determine a system that has the least sensitivity to the fuel's weight. After setting up the machine, the number of trial runs needed to identify the performance of the system could be reduced through simulation, which saves both experimental costs and time. Moreover, tuning the simulation parameters to the announced requirements right before the competition helps to find out the corresponding amount of the fuel. For example, the required traveling distance, load, surface friction, and ambient temperature would be used as the inputs of the simulation to obtain the weight of fuel that should be loaded into the fuel tank.

PROPOSED CAR DESCRIPTION

The performance of a car based on the production of pressurized oxygen from decomposition of hydrogen peroxide will be discussed.

$$2H_2O_2 \xrightarrow{K1} 2H_2O + O_2 \qquad (1)$$

The proposed car consists of a fuel tank, a reaction chamber, and an external load vessel (Figure 1). To maintain a uniform pressure within the system, vessels are connected together by means of a high-pressure hose. The bottom vessel is equipped with a nozzle at one end to let the oxygen exit the system at a high speed. At the beginning of each run, fuel (hydrogen peroxide 30%) is loaded into the fuel tank while the bottom tank contains a little amount of dissolved catalyst (KI). The reaction starts by opening the valve located between two vessels. Decomposition of hydrogen peroxide in the presence of KI solution is an instantaneous exothermic reaction.[5] Due to the short time of each run (~1 min), the heat dissipation to the surroundings is assumed negligible.

The physical and chemical properties of H_2O_2 are obtained from Reference 5, while *Perry's Handbook of Chemical Engineering*[6] was used for all other physical data.

MATHEMATICAL MODEL

To calculate the traveling distance of the car with given specifications, differential displacements of the car should be integrated over the range t = [0, ∞].

$$x = \int_0^{\infty} v_1 dt \qquad (2)$$

Also, by definition, the time derivative of the instantaneous velocity equals to the instantaneous acceleration.

$$a_c = \frac{dv_1}{dt} \qquad (3)$$

There are three distinguishable steps in the movement of the car throughout each run.

- *First, when the pressure is inadequate to create enough thrust force to overcome the static friction, the car remains stationary.*
- *Second, the pressure inside the chamber is high enough to cause a positive resultant force while the fuel is still being consumed.*
- *Third, from the maximum pressure time to the final traveling length. In this step, due to friction, the car's acceleration gradually becomes negative, which finally causes the car to stop.*

$$F = F_t + F_\mu + F_d = \dot{m}_2 v_2 - m_c \mu g + F_d = m_c a_c \qquad (4)$$

$$\dot{m}_2 = \rho_{ox} A_2 v_2 \qquad (5)$$

The magnitude of the drag force, caused by the motion of the car, can be calculated using Eq. (6).

$$F_d = -\frac{\rho_A v_1^2 A_p C_d}{2} \qquad (6)$$

Having a maximum velocity of about 1m/s and a projected area of about 20cm^2, the maximum amount of the drag force is calculated using Eq. (7):

$$F_d = -\frac{1.293\times1\times0.02\times0.3}{2} \approx 0.004\text{N} \tag{7}$$

Comparison of this value with typical values for the friction force (~0.1 N), makes it apparent that the drag force is two orders of magnitude smaller than the frictional forces, and thereby can be neglected.

By substituting Eq. (5) into Eq. (4), it can be seen that the car's acceleration is a function of oxygen velocity and density. The density of oxygen is simply calculated from the following equation.

$$\rho_{ox} = \frac{n_{ox} MW_{ox}}{V} \tag{8}$$

To obtain the number of oxygen moles in the system, a component mass balance is used.

$$\frac{dn_{ox}}{dt} = \frac{\dot{m}_1}{2MW_f} - \frac{A_2 v_2 \rho_{ox}}{MW_{ox}} \tag{9}$$

The velocity of oxygen at the exit nozzle is calculated from Bernoulli's equation.

$$v_2^2 = \frac{4RT(P - P_a)}{MW_{ox} P} \tag{10}$$

Eq. (10) is used to eliminate v_2 from Eqs. (4) and (9). Considering the very fast rate of decomposition of hydrogen peroxide in presence of KI catalyst, the reaction is assumed to be instantaneous. Therefore, the temperature of the system increases due to the heat of reaction.

$$\dot{Q} = \frac{\dot{m}_1 \Delta H}{MW_f} = f_h m_c C_{pc} \frac{dT}{dt} \tag{11}$$

Here, C_{pc} is the weight average specific heat of the car's components and f_h is the weight fraction of the car that is heated due to the heat of reaction. Taking derivatives of both sides of the ideal gas law equation with respect to time, it can be shown that the variation of the inside pressure is due to the simultaneous change in the total number of oxygen molecules and temperature.

$$PV = n_{ox} RT \tag{12}$$

$$\frac{dP}{dt} = \frac{RT}{V}\frac{dn_{ox}}{dt} + \frac{n_{ox} R}{V}\frac{dT}{dt} \tag{13}$$

Equal pressures in the reaction chamber and the fuel tank cause hydrogen peroxide to flow from the top tank to the reaction chamber under gravity. One can calculate the flow rate using Bernoulli's principle and a mass balance on the fuel tank.

$$\frac{\rho_f v_3^2}{2} = \rho_f gL \tag{14}$$

$$\dot{m}_1 = \rho_f v_3 A_1 = \rho_f A_1 \sqrt{2gL} \tag{15}$$

$$\rho_f A_3 \frac{dL}{dt} = -\rho_f A_1 \sqrt{2gL} \tag{16}$$

The variation of the depth of fuel in the fuel tank can be obtained by integrating Eq. (16).

$$\sqrt{L} = \sqrt{L_0} - \frac{A_1\sqrt{2g}\, t}{2A_3} \tag{17}$$

$$L_0 = \frac{m_f}{\rho_f A_3} \tag{18}$$

By substituting the intermediate variables into Eq. (13), the following expression that describes the variation of pressure in the system is obtained.

$$\frac{dP}{dt} = \alpha_1 + \alpha_2 t - \alpha_3 t^2 + \frac{\alpha_4 P}{\alpha_5 + \alpha_6 t - \alpha_7 t^2} - \alpha_8 t - \alpha_9 t^2 + \alpha_{10} t^3 - \frac{\alpha_{11} Pt}{\alpha_5 + \alpha_6 t - \alpha_7 t^2} - P\sqrt{\alpha_{12} + \alpha_{13} t - \alpha_{14} t^2 - \frac{\alpha_{15}}{P} - \frac{\alpha_{16} t}{P} + \frac{\alpha_{17} t^2}{P}} \tag{19}$$

Here, α_1 to α_{17} are positive constants that depend on A_1, A_2, A_3, C_{pc}, ΔH, L_0, MW_f, MW_{ox}, ρ_f, f_h, and T_0. The Runge-Kutta method has been used to solve the differential equations.

RESULTS AND DISCUSSION

The pressure variation inside the system is independent of the car's weight, traveled distance, and friction factor between the wheels and the ground. Therefore, it is possible to analyze the transient pressure of the system regardless of its weight, position and friction factor (Figure 2).

Simulation results indicate that the maximum pressure occurs around the moment when the fuel is completely consumed, and after this moment the pressure inside the chamber starts to decline; this is because no more oxygen is generated while the existing oxygen gradually exits the reaction chamber from the exit nozzle.

After illustrating the variation of pressure with time, the movement of a car with a given weight and friction can be calculated using Eqs. (2) and (3). Expectedly, a great fraction of fuel is consumed just to overcome the initial static friction and to launch the car. After the initial movement, the traveling distance of the car is a strong function of the remaining fuel. Also, simulation demonstrates that the fuel is completely consumed before the car stops. In other words, after passing a specific time, the driving force (produced oxygen) is inad-

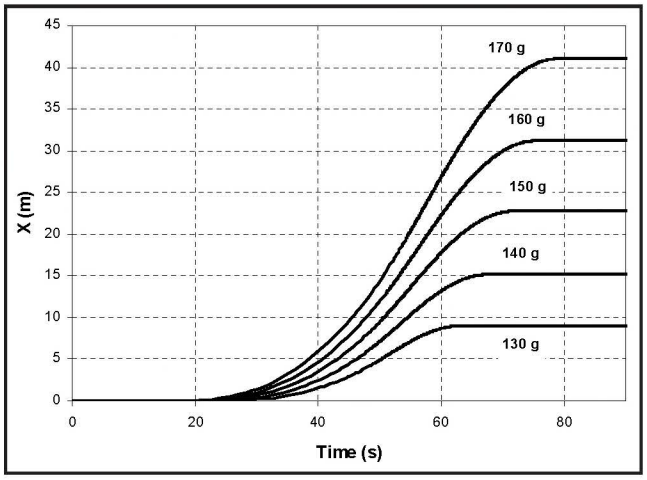

Figure 3. *Distance vs. time for different initial fuel weights, weight of car =750g, μ=0.01, T_0=300 K.*

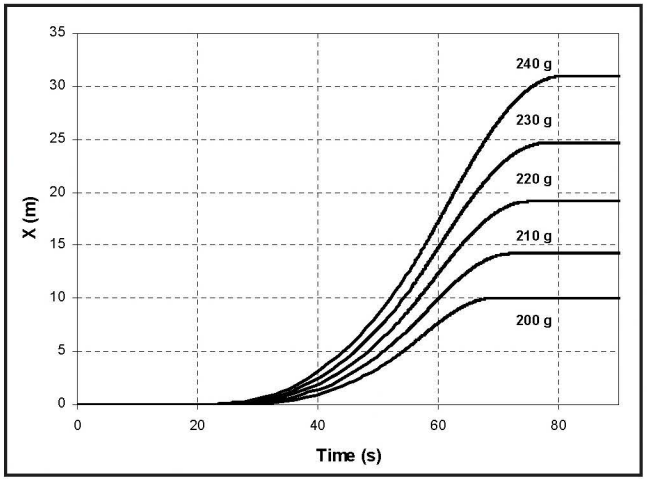

Figure 4. *Distance vs. time for different initial fuel weights, weight of car =1 kg car, μ=0.01, T_0=300 K.*

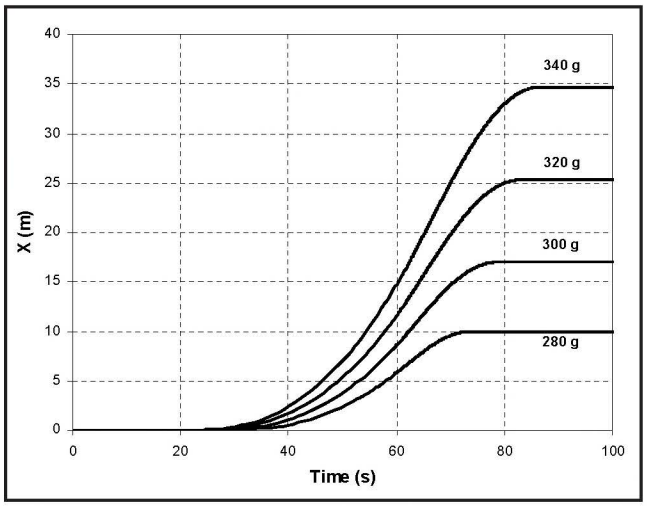

Figure 5. *Distance vs. time for different initial fuel weights, weight of car = 1.25 kg, μ=0.01, T_0=300 K.*

equate to overcome the resistance force (dynamic friction force), which slows down the speed and finally causes the car to stop. (See Figures 3-5.)

To have a more clear picture of the car's performance over the possible ranges of weight, fuel and distance, the contours of iso-distance lines are created using the contour generator in MATLAB (Figures 6 and 7). These figures, or similar figures that are generated and calibrated before the competition, can help determine the appropriate amount of fuel to meet the competition requirements.

SUMMARY

The performance of a hydrogen-peroxide-driven Chem-E-Car was studied using basic engineering principles. The simulation showed that the car stops a few seconds after the occurrence of the maximum pressure inside the system. Also, a noticeable fraction of fuel is consumed to overcome the static friction and, after the very first movement, a little amount of fuel can keep the car moving. In other words, the ultimate traveled distance of the car is very sensitive to the weight of the remaining fuel right after the initial movement. Finally, contours of iso-distance lines are presented for a given friction coefficient and ambient temperature. One can use the same technique to obtain the corresponding contours for different initial conditions. Results are useful for both design purpose and decision making on the day of Chem-E-Car competition.

NOMENCLATURE

A1	Area of fuel supply pipe	m^2
A2	Area of the exit nozzle	m^2
A3	Area of the fuel tank	m^2
a_c	Acceleration of car	m/s^2
A_p	Cross section area of the car	m^2
C_{pc}	Average specific heat of car	J/ kg. K
F_n	Net force	N
C_d	Drag coefficient	-
F_d	Drag force	N
f_h	Mass fraction of car that is heated by the reaction	-
F_t	Thrust force	N
F_μ	Friction force	N
g	Gravity	m/s^2
ΔH	Heat of reaction	J/mol
L	Depth of fuel	m
L_0	Initial depth of fuel	m
$\dot{m}_1$	Fuel mass flow rate	kg/s
$\dot{m}_2$	Oxygen mass flow rate	kg/s
m_c	Overall mass of car	kg
m_f	Initial mass of fuel	kg
MW_f	Molecular weight of fuel	kg/mol
MW_{ox}	Molecular weight of oxygen	kg/mol
n_{ox}	Number of oxygen moles	mol
P	Pressure inside the car	Pa
P_a	Atmospheric pressure	Pa

q	Rate of heat generation	J/s
t	Time	s
T	Temperature	K
T_0	Initial temperature	K
V	Total volume of the fuel tank and reaction chamber	m^3
v_1	Velocity of the car	m/s
v_2	Velocity of oxygen	m/s
v_3	Velocity of fuel	m/s
x	Traveled distance	m
μ	Friction coefficient	-
ρ_f	Density of fuel	kg/m^3
ρ_{ox}	Density of oxygen	kg/m^3
ρ_A	Density of air	kg/m^3

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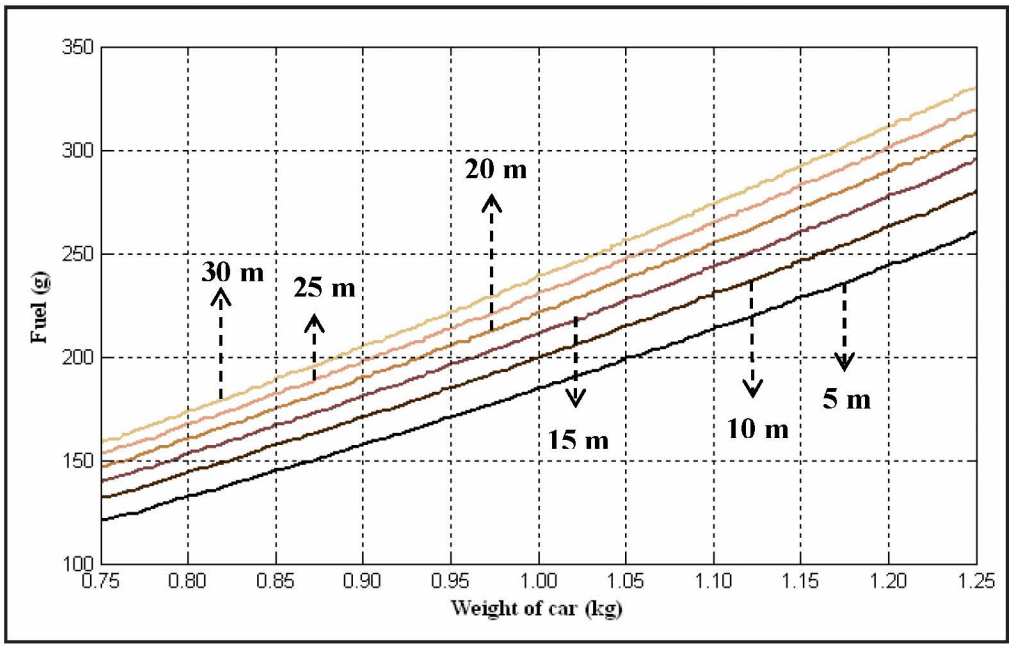

Figure 6. *Contours of iso-distance lines, μ=0.01, T_0=300 K.*

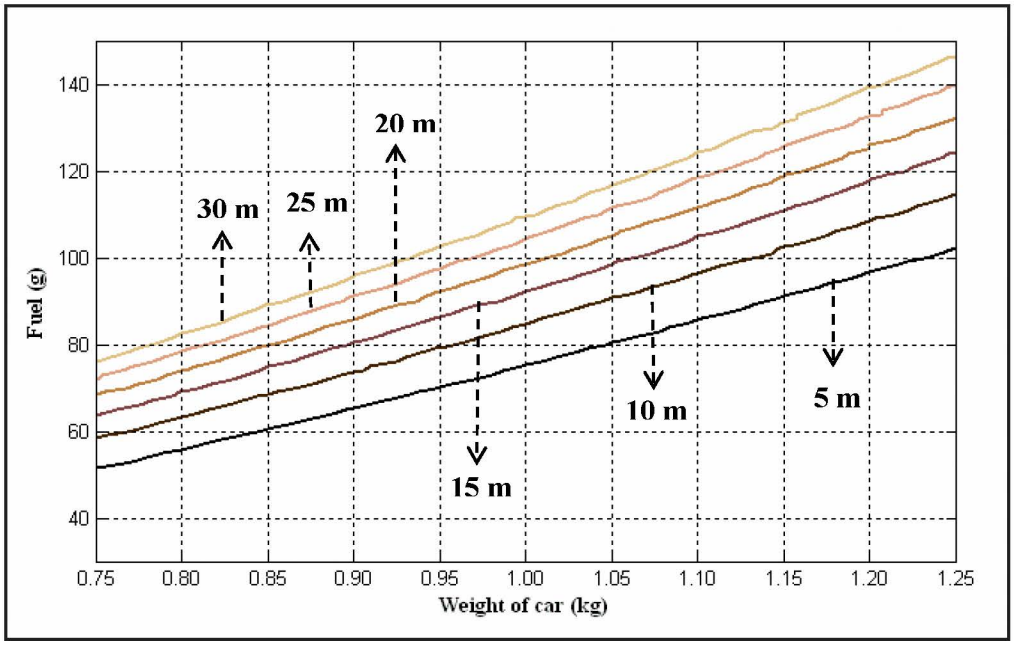

Figure 7. *Contours of iso-distance lines, μ=0.005, T_0=300 K.*