1 Self-Heating Container

Learning Outcomes:

• Apply macroscopic energy balances to physical problems
• Evaluate the feasibility of a proposed engineering solution

OnTech, a San Diego startup company, has developed self-heating containers for meals and beverages. These containers will heat coffee to an optimal drinking temperature of 145°F (63°C) within minutes after pressing a button, and the containers are designed to keep beverages hot for 20 minutes (and warm for about an hour).

When you’re about ready for coffee, turn the can over and remove the “tamper proof foil”. Push the “activation button” to break the “foil seal”. Gravity causes water (“heat generating liquid”) to flow from the “water container” into the “heat generating material”, which is calcium oxide (ρ = 3.34 g/cm³; \( C_p = 42 J/K/mol \)). Water reacts with calcium oxide, producing heat and calcium hydroxide (ρ = 2.21 g/cm³; \( C_p = 87.5 J/K/mol \)):

\[
\text{CaO(s) + H}_2\text{O(l)} \rightarrow \text{Ca(OH)}_2(s); \Delta H_{rxn} = -350 kJ/mol
\]

(The “internal heat generation cone” contains no calcium oxide; it is a finned heat transfer surface that is designed to expedite heat transfer to the coffee by increasing the heat transfer surface area. You may assume that this finned cone requires negligible volume since it’s comprised of very thin, extended surfaces.) After five seconds, turn the can over. Wait about six to eight minutes, pop the top, and enjoy your hot coffee without ever leaving your desk.

You must design a standard 16-oz (470 mL) beverage container to hold coffee and all components of the heat source (water, calcium oxide). Check the feasibility of this concept by calculating the largest volume of coffee that the container can hold while still meeting the requirement that the coffee be heated from room temperature to 145°F (63°C). Does this volume of coffee seem reasonable for a single serving? (You do not need to worry
Figure 1.1: One possible configuration of a self-heating container for meals or beverages, depicting how a liquid could be contained in a disposable device which also has reactants for a highly exothermic reaction. Adapted from diagrams in US Patent US 7117684 B2.

about the rate of heat transfer at this time; so you don’t need to consider the requirement that the coffee reaches 145°F (63°C) in six minutes.)

**Solution**

**Assumptions:**

- Properties of coffee are the same as properties of water
- Internal temperature gradients are negligible at steady state
- Properties of water and calcium oxide do not vary strongly with temperature
- Neglect the heat fins’ thermal mass and volume
- The water and calcium oxide fully react to form calcium hydroxide and were present in stoichiometric quantities
- The reaction volume is exactly the sum of the water and calcium oxide volumes necessary to generate enough heat (i.e. the water exactly permeates the calcium oxide and no additional space is necessary to allow flow of water)
Define variables:

- $\rho_{CaO} = 3340 \text{ kg/m}^3$ is the density of calcium oxide
- $\hat{C}_{p, CaO} = 42 \text{ J/K/mol}/(56.1 \text{ g/mol}) \times (1000 \text{ g/kg}) = 750 \text{ J/K/kg}$ is the per mass heat capacity of calcium oxide
- $MW_{CaO} = 56100 \text{ kg/mol}$ is the molecular weight of calcium oxide
- $\rho_w = 1000 \text{ kg/m}^3$ is the density of water
- $\hat{C}_{p, w} = 4184 \text{ J/kg/K}$ is the per mass heat capacity of water
- $MW_w = 18020 \text{ kg/mol}$ is the molecular weight of water
- $\rho_{Ca(OH)_2} = 2210 \text{ kg/m}^3$ is the density of calcium hydroxide
- $\hat{C}_{p, Ca(OH)_2} = 87.5 \text{ J/K/mol}/(74.1 \text{ g/mol}) \times (1000 \text{ g/kg}) = 1180 \text{ J/K/kg}$ is the per mass heat capacity of calcium hydroxide
- $T_0 = 25^\circ \text{C}$ is the starting temperature (room temperature) of the contents
- $T_f = 63^\circ \text{C}$ is the goal temperature
- $V_c$ is the volume of coffee in the device
- $V_w$ is the volume of water in the device
- $V_{CaO}$ is the volume of calcium oxide in the device
- $V_{react}$ is the volume of the reaction zone in the device
- $V_{Ca(OH)_2}$ is the final volume of the calcium hydroxide (not necessarily the same as $V_{react}$)
- $V_{tot} = V_c + V_w + V_{react} = 470 \text{ mL}$ is the total volume of the interior of the device
- $\Delta \hat{H}_{\text{rxn}} = -350 \text{ kJ/mol}/(56.1 \text{ g/mol}) \times (1000 \text{ g/kg}) \times (1000 \text{ J/kJ}) = -6.2 \times 10^6 \text{ J/kg}_{CaO}$ is the heat of reaction of calcium oxide and water on a calcium oxide mass basis

Setting up the macroscopic balance on the whole device (or you can do it control volume by control volume): Accumulation = In - Out + Generation - Consumption.

The accumulation term contains the change in temperature of the water, calcium oxide, and coffee. There is no net in and out for the whole device. The generation term is the reaction of the calcium oxide and water, which we will denote as a source term $S$.  

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Mathematically, that looks like:

\[
\frac{d}{dt} \int_V \rho \hat{C}_p T \, dV = \int_V S \, dV \tag{1.1}
\]

There are two volumes of interest—the coffee and the reaction volume (the combination of the water and calcium oxide). Assuming uniform properties within each volume and that \( S \) is zero in the coffee and non-zero in the reaction volume, Equation \( \tag{1.1} \) becomes:

\[
\frac{d}{dt} (\rho_w \hat{C}_{p,w} V_c + \rho_{react} \hat{C}_{p,react} V_{react}) T = V_{react} S \tag{1.2}
\]

Integrating both sides with respect to time, the right hand side becomes the heat of reaction times the initial mass of calcium oxide:

\[
(\rho_w \hat{C}_{p,w} V_c + \rho_{Ca(OH)2} \hat{C}_{p,Ca(OH)2} V_{Ca(OH)2}) T_f
- (\rho_w \hat{C}_p V_c + \rho_{CaO} \hat{C}_{p,CaO} V_{CaO} + \rho_w \hat{C}_{p,w} V_w) T_0 = \]

\[ - \Delta \hat{H}_{rxn} \rho_{CaO} V_{CaO} \tag{1.3} \]

The volume of calcium hydroxide at the end is related to the volumes of water and calcium oxide at the start by conservation of mass:

\[ \rho_w V_w + \rho_{CaO} V_{CaO} = \rho_{Ca(OH)2} V_{Ca(OH)2} \tag{1.4} \]

The volumes of water and calcium oxide are related by stoichiometry:

\[ \rho_w V_w / MW_w = \rho_{CaO} V_{CaO} / MW_{CaO} \tag{1.5} \]

The volumes are all related by:

\[ V_{tot} = V_c + V_w + V_{react} = V_c + 2V_w + V_{CaO} \tag{1.6} \]

Our unknowns are: \( V_{Ca(OH)2} \), \( V_w \), \( V_c \), \( V_{CaO} \). We thus have 4 equations and 4 unknowns.

Solving using your favorite software package for systems of linear equations, we obtain that the volumes are 460 mL for the coffee, 3.7 mL of water to react, and 3.5 mL of calcium oxide, which will form 6.9 mL of calcium hydroxide (which fits in our reaction volume). Because the heat fins were neglected and other assumptions, this estimate is the best case scenario, but it does bode well. The coffee is the majority of the 470 mL volume, which means it is a very reasonable serving.