FEB 28 1995

Mr. Ralph A. Simmons
Law Offices
Keller and Heckman
1001 G Street, N.W.
Suite 500 West
Washington, DC 20001

Re: Food Additive Master File No. 518

Dear Mr. Simmons:

This is in further response to your letter of May 13, 1994, requesting clarification of our decision to limit the use of Continental's (Continental P.E.T. Technologies, Inc.) post-consumer polyethylene terephthalate (PET) to a storage period not to exceed one year. The recycled PET would be used to manufacture tri-laminated PET bottles consisting of a thick inner and outer layer of virgin PET, complying with 21 CFR 177.1630, that sandwich a core layer of thick post-consumer PET. The PET bottles are intended to hold aqueous, acidic, and low-alcoholic foods under Conditions of Use C (Hot filled or pasteurized above 150°F (66°C)) and below.

Our letter of August 15, 1994, stated that our decision for the limitation of a one year storage period was based on our reviews of the data you provided in Food Additive Master Files 518 and 553, and the following assumptions and equations:

1. Migration across an uncontaminated layer is modeled by assuming that the concentration of contaminant in the recycled polymer remains constant and that the food is an infinite sink for the contaminant., both conservatisms;

2. A dietary concentration of up to 0.5 parts per billion (ppb) is an acceptable limit for unregulated substances that might migrate from recycled PET (consistent with currently proposed threshold of regulation);

3. Heavily contaminated PET can be washed to leave no more than 100 ppb of contaminant, as shown by data submitted in your FAMF 553; and

4. All recycled PET resins are contaminated at the 100 ppb level and 100 percent recycled PET is used as the non-food-contact layer.

The assumption that the recycled layer is an infinite source of contaminants is the main limitation of the diffusion model. In reality, the concentration of contaminant would decrease with time in the recycled layer as it increases in the virgin layer and, finally, in the food.

The equation below (Equation 1) is the principal equation relating diffusion coefficient and migration:

$$M_t = 2C_0\sqrt{\frac{Dt}{\pi}} \qquad (1)$$

where M_t is the migration from the polymer (in g/cm^2) at time t (in s), C_0 is the initial concentration of the migrant in the polymer (in g/cm^3), and D is the diffusion coefficient (in cm^2/s) of the migrant in that polymer. This equation has been used successfully for many years to predict migration of additives and other substances from polymers into food (or food simulants).

Equation 2 (below) was shown by Begley and Hollifield (*Food Technology*, November 1993, pp. 109 - 112) to be useful for estimating migration into food of a contaminant present in the non-food-contact layer (made of recycled plastic) of a laminated package structure, where a virgin layer of polymer, with a thickness l, serves as the food-contact layer:

$$M_t = \left[\frac{Dt}{l^2} - \frac{1}{6} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\exp\left(\frac{-Dn^2\pi^2 t}{l^2}\right)\right]C_0 l \qquad (2)$$

For long time periods (as $t \rightarrow \infty$) this equation simplifies to (see *The Mathematics of Diffusion*, J. Crank, Clarendon Press, Oxford, p. 51, eq. 4.25) :

$$M_t = D \times \frac{C_o}{l} \times \left(t - \frac{l^2}{6 \times D}\right) \qquad (3)$$

This is the form of the equation that we used to arrive at our decision to limit the use of Continental's PET tri-laminated bottles to a storage period not to exceed one year.

Equation 4 (below), a more refined version of Equation 2 that accounts for diffusion through the thickness of the recycled layer, will give a better estimate of migration through a virgin layer with thickness l covering a recycled layer of thickness l_R:

$$M_t = \left[\frac{Dt}{l^2} - \frac{1}{6} - \frac{2}{\pi^2}\sum_{n=1}^{\infty}\frac{-1^n}{n^2}\exp\left(\frac{-Dn^2\pi^2 t}{l^2}\right)\right] l C_0 \left[2\sqrt{\frac{Dt}{l_R^2\pi}}\right] \qquad (4)$$

All of these equations must be used cautiously. They are limited by the assumptions used in their derivation. We have recently explored some of the assumptions and have demonstrated that the calculations will break down under certain conditions. Some useful steps for assessing migration from laminated packaging, while emphasizing the limitations of these equations, are:

1) Calculate the maximum amount of migration (M_{max}) that can occur assuming 100% of a monomer, additive or contaminant enters the food.

2) Calculate the value τ for the bulk package thickness (τ_m, generally 10 - 20 mil) and for a virgin layer thickness (τ_v) if a virgin layer is going to be placed over recycled polymer.

$$\tau = \frac{Dt}{l^2}$$

As can be seen, the expression Dt/l^2 appears in equations 2 and 4. By defining τ in this manner, these equations are simplified and become more useful in evaluating diffusion and migration. The value of τ is an indication of the extent of the diffusion process for the intended conditions (time and temperature) of use. The larger the value of τ, the greater the diffusion.

3) For a single-layer container, use Equation 1 to estimate migration when $\tau_m < 0.2$. If $\tau_m > 0.2$, then 100% migration should be assumed.

4) For a layered package, use Equation 2 to estimate migration if τ_v is less than 1.5. Results from Equation 4 and Equation 3 (which is from Equation 2) should be compared with 100% migration calculations when $\tau_v > 1.5$.

In the calculations performed for FAMF 518, $\tau_m = 0.12$, but $\tau_v = 49$. Our calculations for Continental's post-consumer laminated bottles did not recognize the effect of τ_v on the outcome of the calculations, in addition to neglecting to perform Step 1. Because τ_v is so large, the use of Equation 3, which led to the conclusion that there should be restrictions on use conditions, was not appropriate. Rather, the approach used in the "Points to Consider" document (assuming 100% migration of the contaminant) is the most appropriate for this system. In this case, a 100 ppb contaminant level would result in a dietary concentration of only 0.2 ppb. Therefore, no restrictions on the conditions of use or time of storage for the Continental bottle (with a sidewall of virgin food-contact layer over a recycled core) are necessary.

If I can assist you further, please let me know.

Sincerely yours,

/s/

Eugene C. Coleman
Director
Division of Petition Control
Center for Food Safety
and Applied Nutrition