# MODELLING THE 5–30 $\mu$m SPECTRUM OF COMET HALLEY

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**Abstract.** The 5–30 $\mu$m spectrum of Comet P/Halley is modelled for various grain compositions on the basis of an observationally determined distribution of grain sizes. We compute the distribution function of grain temperatures and fluxes arising from (1) a mineral grain model, and (2) an organic grain model comprised of a diatom/POM mixture. The organic/POM model yields excellent accord with the cometary observations.

A composite spectrum of Comet P/Halley combining data over the wavelength range 16–30 $\mu$m with observations in the range 5–14 $\mu$m is shown by the points in Figure 1 (Herter *et al.*, 1987). In the present communication we attempt to model this data in terms of various candidate materials for cometary grains. The relevant data over the 16–30 $\mu$m waveband were obtained on 14 December 1985 (Herter *et al.*, 1986) whilst the data over the shorter wavelength band was obtained on the adjacent dates 12 and 13 December 1985) (Bregman *et al.*, 1986; Tokunaga *et al.*, 1986). The combination is dependent on a single overlapping point at 20 $\mu$m. The average heliocentric distance when all these observations were made was $\sim 1.32$ AU.

At a distance of 1.32 AU absorbing particles with dimensions large compared with infrared wavelengths would take up a temperature equal to the effective black-body temperature in the solar radiation field, $\sim 250$ K. Smaller particles will in general take up temperatures that depend upon the detailed properties of the $Q_{abs}(\lambda)$ curve over both the visual and infrared wavebands. For particles that include a significant free carbon content whose largest dimension satisfies the condition $2\pi a/\lambda \gg 1$ for the longest relevant infrared wavelengths, we expect emission corresponding to a temperature of $T \cong 250$ K. A cloud of smaller particles, optically thin as in Halley, would on the other hand give rise to a spectrum determined essentially by the distribution of grain temperatures and the emissive properties of individual particles. Small grains are generally hotter than thermal, and Hanner (1983) found that summing emissions from a distribution of grains gives a mean curve 'hotter' than black body and with an excess flux at wavelengths above 15 $\mu$m.

Herter *et al.* (1987) chose to model the data of Figure 1 using an hypothetical 'silicate' spectrum derived from circumstellar IR sources combined with an independent black-body distribution. We consider instead a realistic model involving a combination of a black-body spectrum and emission from an optically thin distribution of grains comprised of real materials. The curves in Figure 1 show normalised Planck distributions at various temperatures ($T = 250$, 270 and 300 K). Although

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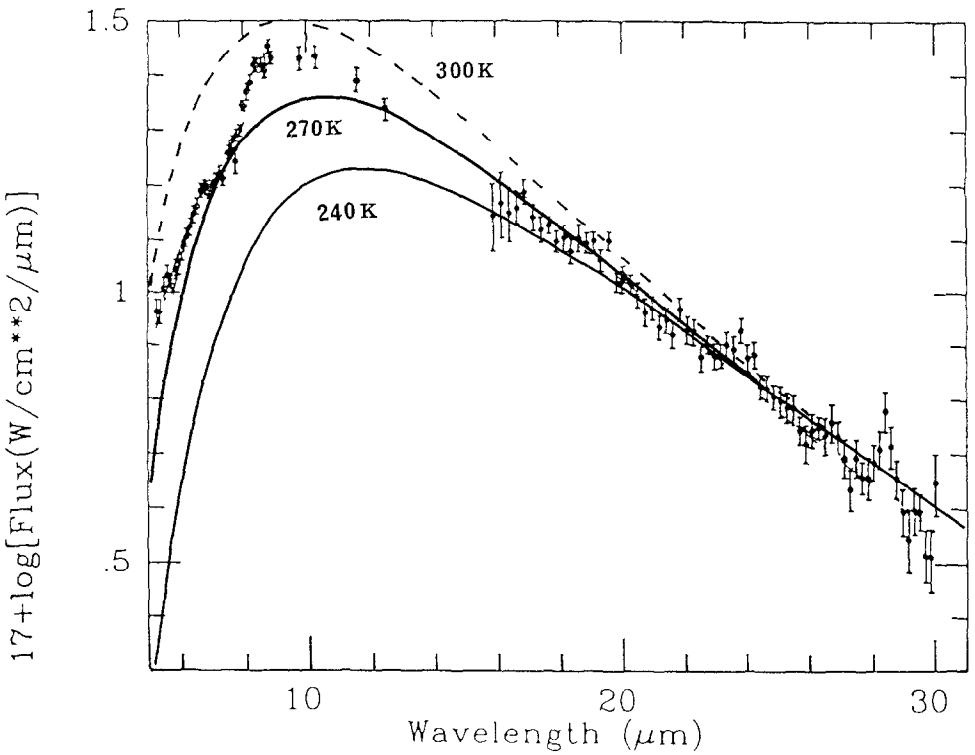


Fig. 1. Composite spectrum of Comet Halley on December 12–14, 1985 compared with normalised Planck distributions.

the curve for $T = 270$ K gives rough agreement over the entire 5–30 $\mu$m waveband the detailed correspondence over the shortwave end of the spectrum and at the peak is poor. Nor could any other single temperature of a black body improve the overall fit. From Figure 1 it is clear that an emission feature centred at 10 $\mu$m exists, and also other less prominent features in the 6–7 $\mu$m waveband and possibly in the further infrared (23.5, 28.5 $\mu$m).

Previous cometary IR observations involved broad-band ($\sim 1$ $\mu$m) photometry (Ney, 1974; Campins and Hanner, 1982). The new data on Comet Halley is a substantial improvement and would permit discrimination between competing models. The excess 10 $\mu$m emission is usually ascribed to a small fraction of silicates, which have to be either amorphous or hydrated in order to produce such a broad feature (Hanner, 1983). Disordered olivine has been favoured to explain Ney's data from comet Kohoutek, which includes a feature corresponding to an apparent excess at 18 $\mu$m. However, the absence of a strong 18 $\mu$m excess in the Comet Halley data may be interpreted as casting doubt on a silicate identification.

We investigate two broad classes of grain model:

(1) Mineral particles with a free carbon content of $\sim 8\%$ by volume, representing carbon-rich chondritic-type material.

(2) Organic particles (including diatoms) which may be taken to be partially graphitised to the extent of $\sim 0.8\%$ by volume.

For models in class (1) we use tabulated $n$, $k$ values in the infrared as given by Bromage *et al.* (1973) for andesite, and in the visual and ultraviolet spectral regions we use data for olivine given by Huffman and Staff (1973). For particles in class (2) we use values appropriate for POM (polyoxymethylene, heated to 170 K) to represent a polymer in a state of partial degradation as given by Cook (1973) who used the data of Todokoro *et al.* (1963). For diatoms we use Al-Mufti's (1985) measurements of infrared wavelengths from which $k(\lambda)$ is computed from the relation

$$k(\lambda) = \alpha\lambda/(4\pi); \tag{1}$$

at visual and ultraviolet wavelengths we use data appropriate for biomaterial including diatoms as given by Yabushita *et al.* (1987). The infrared $n(\lambda)$ values for diatoms are computed using the Kramers-Krönig equations. For each type of organic-graphite system we take the average $\bar{n}$, $\bar{k}$ values to be given by

$$\left.\begin{aligned} \bar{n} &= 1 + (1-f)(n_s - 1) + f(n_G - 1), \\ \bar{k} &= (1-f)k_s + fk_G; \end{aligned}\right\} \tag{2}$$

where $n_s$, $k_s$ refer to values corresponding to either diatoms or POM, and $n_G$, $k_G$ are the values for graphite as given by Taft and Phillipp (1965). Here $f$ denotes the volume fraction of graphite included along with the organic material. For all our model calculations we adjusted $f$ so that 1/3 of the $\bar{k}(\lambda)$ values at $\lambda = 9\ \mu$m arose from graphite. For such a mixture the $\bar{k}(\lambda)$ values in the visual and ultraviolet spectral regions are dominated by the properties of graphite. Table 1 shows the values of $k_s(\lambda)$ for POM, diatoms and andesite that were used in our calculations. These values turn out to be crucial in distinguishing one model from another in relation to the detailed profile of the 5–14 $\mu$m absorption.

We adopt a size-distribution of organic grains given by

$$n(a)\mathrm{d}a = \text{const.}\ \frac{\mathrm{d}a}{a^{3.6}}, \quad a \geqslant 0.5\ \mu\text{m}, \tag{3}$$

which is known to be consistent with the data for Comet Halley (McDonnell *et al.*, 1986, 1987). To calculate the emitted infrared flux from such a distribution of particle sizes we first calculate an equilibrium grain temperature for each value of radius $a$, assuming a detailed balance of solar radiation absorbed at 1.3 AU and the emitted infrared flux. For the purpose of this calculation we assume that the particles are all spherical and we compute $Q_{abs}(\lambda)$ values from the Mie formulae using $\bar{n}$, $\bar{k}$ values given by equation (2).

TABLE I

Values of $k$ in the range 5–14 $\mu$m

| $\lambda(\mu)$ | Andesite | Diatoms | POM |
|---|---|---|---|
| 5 | 0.01 | 0.005 | 0.001 |
| 5.3 | 0.01 | 0.006 | 0.002 |
| 5.6 | 0.01 | 0.006 | 0.005 |
| 5.9 | 0.01 | 0.010 | 0.005 |
| 6.2 | 0.01 | 0.014 | 0.010 |
| 6.4 | 0.015 | 0.013 | 0.010 |
| 6.6 | 0.02 | 0.013 | 0.011 |
| 6.8 | 0.025 | 0.014 | 0.015 |
| 7.2 | 0.03 | 0.018 | 0.012 |
| 7.5 | 0.05 | 0.018 | 0.011 |
| 7.7 | 0.08 | 0.019 | 0.012 |
| 8.0 | 0.11 | 0.027 | 0.018 |
| 8.3 | 0.18 | 0.038 | 0.031 |
| 8.6 | 0.33 | 0.049 | 0.049 |
| 9.0 | 0.85 | 0.080 | 0.082 |
| 9.2 | 0.89 | 0.086 | 0.075 |
| 9.5 | 0.92 | 0.089 | 0.073 |
| 10.0 | 1.1 | 0.089 | 0.086 |
| 10.2 | 1.04 | 0.065 | 0.098 |
| 10.5 | 0.86 | 0.052 | 0.115 |
| 11.0 | 0.42 | 0.035 | 0.105 |
| 11.5 | 0.2 | 0.023 | 0.063 |
| 11.7 | 0.17 | 0.022 | 0.051 |
| 12.0 | 0.13 | 0.024 | 0.047 |
| 12.5 | 0.11 | 0.030 | 0.010 |
| 13.0 | 0.09 | 0.032 | 0.008 |
| 13.5 | 0.10 | 0.032 | 0.001 |
| 14.0 | 0.11 | 0.030 | 0.001 |

The emitted flux from our assumed size distribution of grains is then given by

$$F_\lambda \propto \int_{0.5\ \mu\mathrm{m}}^{\infty} B_\lambda(T) Q_{abs}(\lambda) \frac{\mathrm{d}a}{a^{3.6}}, \tag{4}$$

where $B_\lambda(T)$ is the Planck function and $T = T(a)$ is a function of radius which was previously calculated. At infrared wavelengths the usual asymptotic expressions instead of the Mie formulae are used for $Q_{abs}(\lambda)$. For practical purposes we truncate the integral in (3) at an upper limit of 50 $\mu$m. Computed results are found insensitive to this value of the upper limit. Our chosen value corresponds to masses of about 1 $\mu$g above which the McDonnell *et al.* (1986) data deviates above the spectrum (3). Particles larger than this may contribute significantly and are represented by a 'black-body' spectrum which is added as a separate component. The final $F_\lambda$ curve combining these two components is normalized to fit the observations near 9 $\mu$m.

For all the cases we have considered here the computed temperatures turned out to be a slowly decreasing function of grain radius in the range $a \sim 0.5$ to 3 $\mu$m, with

an average value in the range 360–390 K. The flux computed from Equation (4) over the spectral range 5–14 μm was always well represented by a single temperature close to 370 K with $F_\lambda \sim B_\lambda(370)Q_{abs}(\lambda)$, but significant deviations from this behaviour occurred for $\lambda \gtrsim 18$ μm. The computed flux curves were found to be insensitive to the precise value of the lower limit near 0.5 μm of the integral in Equation (4), and also to the index of the power law in the distribution of particle sizes as long as the latter was in the range 3.5–4.

For a silicate model including an 8% volume concentration of carbon in the form of graphite, our computed normalised flux curves in the 5–14 μm waveband are plotted in Figure 2a. The points are the 12 December 1985 observations of Bregman *et al.* (1987). The curve marked 0 is for a flux not augmented by a thermal background at $T = 250$ K. The curves marked 0.25, 0.5 include a contribution from a 250 K black-body amounting respectively to 1/5 and 1/3 of the total flux at 9 μm. It is clear from this figure that no silicate based grain model of the type considered here could fit the detailed width and shape properties of the 8–12 μm band as observed by Bregman *et al.* (1987). In Halley as in other comets crystalline silicates give a far narrower feature than that observed. Since a substantial fraction of mineral grains were in fact detected by the Halley probes, the present considerations would seem to imply that they were largely 'outshone' in their 10 μm emission. Such

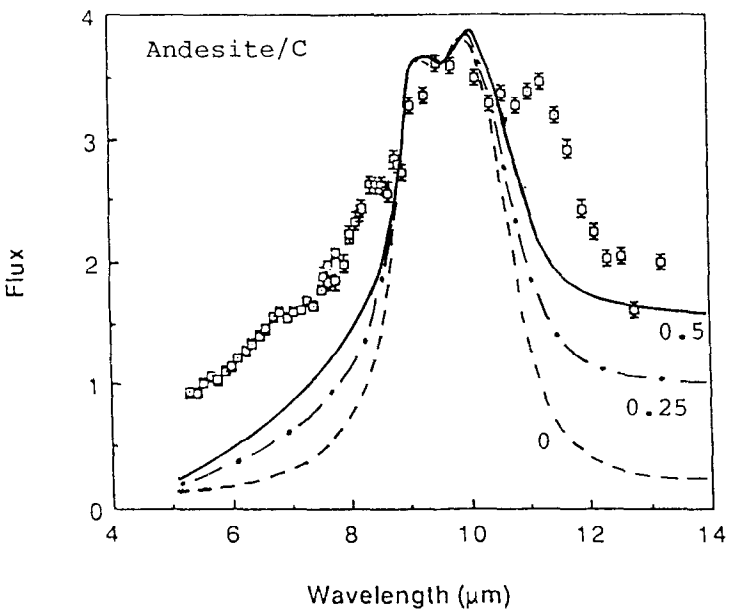


Fig. 2a. Normalised flux from grains comprised of andesite with a 8% by volume carbon content. Several curves correspond to 250 K black-body contributions amounting to 0, 1/5 and 1/3 of the total flux at 9 μm. The points are the observational data of Bregman *et al.* (1987) for 12 December 1985. (One point at 9.7 μm is omitted because of miscorrection for atmospheric ozone.)

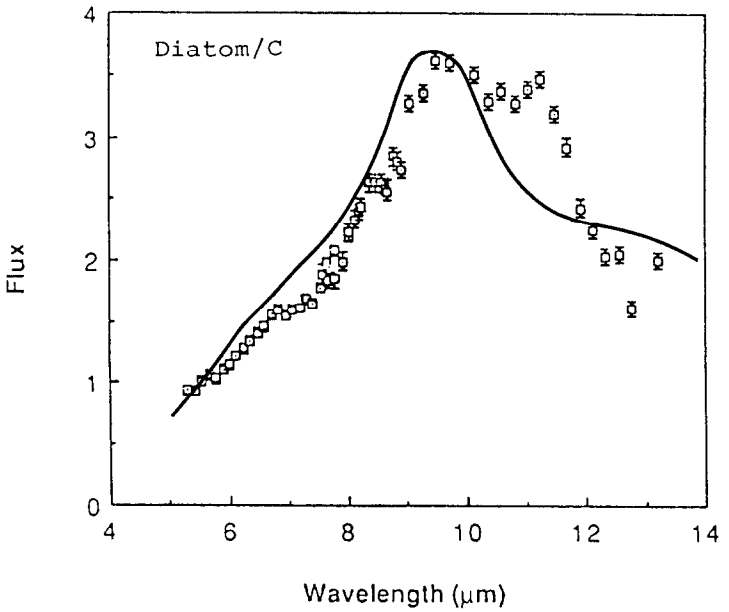


Fig. 2b. Normalised flux from a diatom grain model including an 0.8% by volume carbon content. A 250 K black-body is added, amounting to 1/3 of the flux at 9 $\mu$m. The points are the observational data of Bregman *et al.* (1987) for 12 December 1985.

a situation could arise for relatively pure mineral grains which have no absorption bands in the visual and near ultraviolet wavebands. Small mineral grains would then take up temperatures considerably less than 250 K that are too low for them to be detected in the 8–12 $\mu$m band within the framework of our composite model which includes a large fraction of hotter organic grains.

An alternative non-silicate model for the 10 $\mu$m cometary feature which was originally observed in Comet Kohoutek (Ney, 1974) was proposed by Vanýsek and Wickramasinghe (1975). At that time we considered the possibility of polyoxymethylene (POM) grains. This proposal has recently received a measure of support from an analysis of data obtained from the heavy-ion analyser PICCA aboard the Giotto satellite. The instrument recorded mass peaks corresponding to 61, 75, 91 and 105 AMU which Huebner (1987) and Mitchel *et al.* (1987) have attributed to fragments of polyoxymethylene (POM).

Although we originally conceived that variants of these polymers are the primary component of cometary grains, an alternative source of such linear polymers could be from pyrolysis of biomaterial such as sporopollenin (Rouxhet *et al.*, 1979). For models of class (2) in the present discussion we consider combinations of biological particles typified by diatoms (Hoyle *et al.*, 1982), along with polyoxymethylene polymers in various proportions. In both types of material we postulate a volume fraction of graphitic material amounting to 0.8%, contributing to 1/3 of the

absorption coefficient at $\lambda = 9\ \mu$m. The curve in Figure 2b shows the calculated spectrum for diatoms which agrees with the data points to a slightly better degree than our silicate model. These calculations again include a 1/3 contribution from a 250 K thermal background at $\lambda = 9\ \mu$m. The solid curve in Figure 3 is for pure POM and the dashed curve is for a mixture of diatoms and POM contributing equally to emission at 9 $\mu$m. These two models, particularly the POM curve, provides a good match to the observational data of Bregman *et al.* (1987).

In Figure 4 we show the spectrum over the entire 5–30 $\mu$m band for both the diatom (solid curve) and the POM model. The closeness of the overall fit would give substantial credibility to these models. The POM might arise from thermal degradation of diatom-type material, while polysaccharide variants might well improve the detailed fit. While the fit of Herter *et al.* (1987) might be construed as being of similar quality, ours has advantage in using real rather than synthetic 'astronomical' spectral data for the broad 8–12 $\mu$m emission and in using organic solid material as actually detected by the Halley spacecraft. Further work, particularly aimed at reproducing the 23.5 and 28.5 $\mu$m features should discriminate between the organic and mineral grains models. These latter structures might arise if a fraction of our 'black-body emitters' at 250 K included degradation products of organic polymers with residual spectral features in the 20–30 $\mu$m waveband.

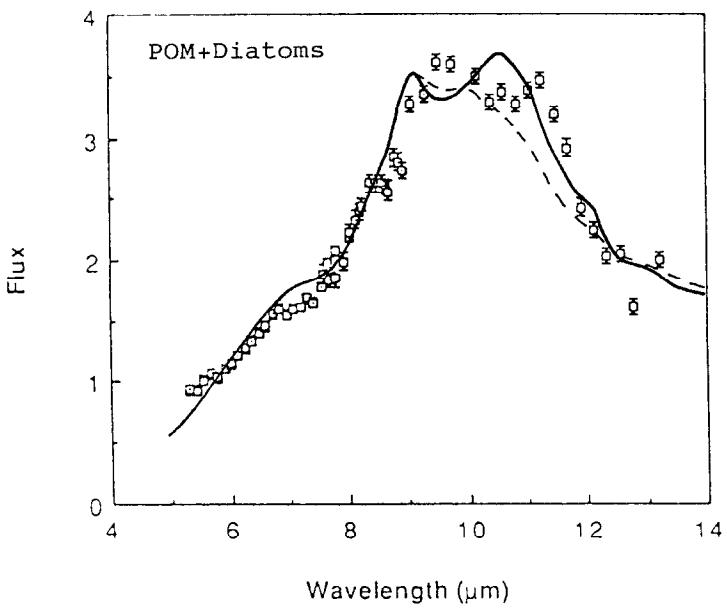


Fig. 3. Normalised flux from a POM grain model including a 0.8% by volume carbon content (solid curve), and from a POM/diatom mixture contributing equally to the flux at 9 $\mu$m (dashed curve). In each case a 250 K black-body spectrum is added amounting to 1/3 of the total flux at 9 $\mu$m. The points are the observational data of Bregman *et al.* (1987) for 12 December 1985.

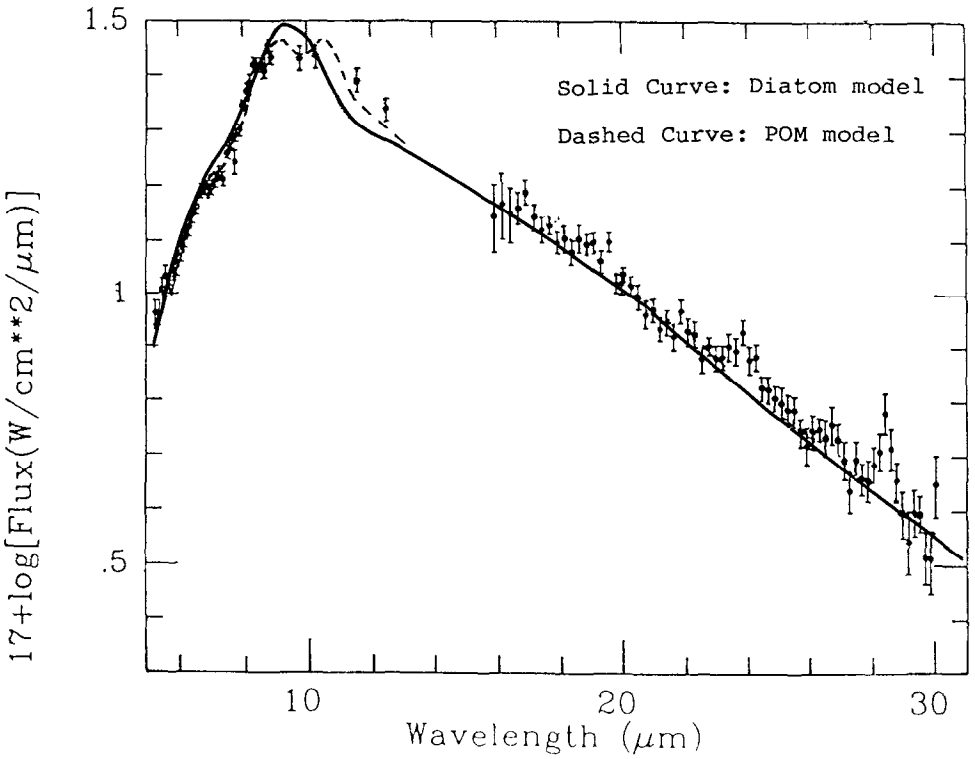


Fig. 4. Normalised flux curves for the 5–30 $\mu$m spectral region. The solid curve is for a diatom model augmented by a 250 K black-body amounting to a 1/3 contribution to the total flux at 9 $\mu$m. The dashed curve represents modification for a POM grain model.

## Note added in Proof

Data over the 6–12 $\mu$m wavelength region secured from the Vega comet probe at 0.8 AU (Combes *et al.*: 1988, *Icarus*, in press) shows a double peaked spectral feature over the 9–11.5 $\mu$m waveband, very similar to the situation shown in Figures 2 and 3. This confirms that the feature is independent of atmospheric corrections and is a persistent characteristic of the dust in Halley's comet.

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