COUPLED ESCAPE PROBABILITY FOR AN ASYMMETRIC SPHERICAL CASE: MODELING OPTICALLY THICK COMETS

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ABSTRACT

We have adapted Coupled Escape Probability, a new exact method of solving radiative transfer problems, for use in asymmetrical spherical situations. Our model is intended specifically for use in modeling optically thick cometary comae, although not limited to such use. This method enables the accurate modeling of comets' spectra even in the potentially optically thick regions nearest the nucleus, such as those seen in *Deep Impact* observations of 9P/Tempel 1 and *EPOXI* observations of 103P/Hartley 2.

Key words: comets: general - methods: numerical - opacity - radiative transfer

Online-only material: color figures

1. INTRODUCTION

Comets are understood to be frozen remnants from the formation of our solar system. As such, their chemical composition is of great significance to understanding the origin of the planets and the distribution of important molecules, including water, throughout the solar system. This was and is a major goal of the *Deep Impact* and *EPOXI* missions, among others, as well as ground-based observations of comets.

Recent observations, in particular those of the Deep Impact and EPOXI missions (see, e.g., Feaga et al. 2007; A'Hearn et al. 2011), have provided better spectra of a cometary coma than were, in general, previously available. These observations include spectra with high spatial resolution very near to the nucleus. Most ground-based observations until the very recent past did not have spatially well-resolved spectral data, and thus there was little observationally driven need to pay special or close attention to the densest part of the coma. Earlier groundbased observations could only see optically thick regions of comae for the brightest and/or most active of comets (e.g., Hale Bopp; see DiSanti et al. 2001; Bockelée-Morvan et al. 2010). Even today, much long-slit spectroscopy often tries to rely on the part of the coma at larger projected distances ($\sim 10^3 - 10^4$ km) beyond the likely influence of optical thickness for determining production rates, thus obviating the need for a careful treatment of optical depth effects.

Therefore, many earlier studies that modeled spectra of comae, in keeping with the available observations of the time, did not attempt to calculate optical depth effects on spectra. Optically thin comae were assumed, since the field of view in those observations being modeled would be dominated by the majority of the coma far from the nucleus, which is optically thin (see, e.g., Chin & Weaver 1984; Crovisier & Le Bourlot 1983). However, with the proliferation of space missions to comets, as well as much better instruments for ground-based observations (see, e.g., DiSanti et al. 1999), this is no longer a truly tenable approach.

Our goal is to better understand the abundances, distributions, and creation mechanisms of various gases observed in comae, in particular of comet 9P/Tempel 1, the target of the *Deep Impact* mission, and 103P/Hartley 2, the subject of the *EPOXI* mission.

In order to do so, we have built a computer model of the spectrum of the comet's coma that includes the difficult and often ignored problem of accurately including radiative transfer to account for the potentially optically thick coma (or regions of the coma) near the nucleus.

This model will facilitate analyzing the actual spectral data from the *Deep Impact* and *EPOXI* missions to better determine abundances of key species, including CO, CO_2 , and H_2O , as well as remote sensing data on active comets.

1.1. The Simple Coma Model

We begin our modeling of IR rovibrational spectra of a coma by initially following the method used by Chin & Weaver (1984), Crovisier (1987), and others with some minor improvements. As in those models, we assume a constant expansion velocity, thus linearly relating any radial distance to a specific time since a "parcel" of gas was released from the surface of the nucleus. Therefore, we numerically integrate over time the linear differential equations defined by the Einstein coefficients and collisional rate coefficients to get fractional molecular energy level populations for each distance from the nucleus, from which we calculate emission spectra:

$$\frac{dn_k}{dt} = \sum_i (A_{ik}n_i + J_{\nu_{ik}}(B_{ik}n_i - B_{ki}n_k)) + \\
- \sum_l (A_{kl}n_k + J_{\nu_{kl}}(B_{kl}n_k - B_{lk}n_l)) \\
+ \sum_i C_{jk}(n_k - n_j e^{-E_{jk}/k_BT}).$$
(1)

Here *i*, *j*, *k*, and *l* indicate energy levels of a molecule, with the *n*'s with those indices being the corresponding level populations. The Einstein coefficients between levels *x* and *y* are A_{xy} and B_{xy} , and *C* is a similar collisional coefficient. We use $J_{v_{xy}}$ for the mean intensity of radiation at the frequency corresponding to the transition between *x* and *y*, E_{xy} is the energy difference between levels *x* and *y*, and k_B and *T* have their usual meanings. The summations are over all levels *i*, *l*, or *j* that have a transition into or out of level *k*. For collisional coefficients $C = n_{H_{20}} \sigma \bar{v}$, where $n_{H_{20}}$ is the number density of H₂O (assumed to be the dominant collisional partner), σ is the collisional cross section for a given transition, and \bar{v} is the mean (thermal) molecular speed. This allows us to include a timevariable production rate. We use such a coma integration as



Figure 1. Temperature profile of cometary atmosphere based on Combi (1989) for surface temperature of 200 K and radial gas velocity of 0.8 km s^{-1} .

the initial basis for our coma model before including potential optical depth effects.

Although this simple approach to expansion velocity is not strictly accurate near the nucleus (where the gas is undergoing acceleration before reaching a constant velocity), it is a commonly used approximation in conjunction with a Haser model and is often relied on by cometary scientists (e.g., to derive production rates). For the majority of the observations modeled here as hypothetical examples, it should be a sufficiently reasonable approximation, since most of the modeled observations are farther from the nucleus than the extent of major acceleration (see, e.g., Tenishev et al. 2008). In future modeling, this approximation can be replaced with a more accurate treatment for modeling *Deep Impact* observations of the very innermost comae of comets Tempel 1 and Hartley 2.

Our primary improvement is the inclusion of radiative transfer calculations using our spherical adaptation of the Coupled Escape Probability method (hereafter "CEP"; see Elitzur & Asensio-Ramos 2006, hereafter, "CEP06") to more correctly model optically thick (or potentially thick) regions of cometary comae. This is described in detail below and is the main part of this paper. We use the coma integration results to provide the "initial guess" values for populations used in the subsequent radiative transfer calculations using CEP.

For the purposes of the initial coma model, we treat the comet as spherically symmetric and as having a uniform and constant gas production rate over its entire surface. The outward speed of the gas is also assumed to be constant, as in Chin & Weaver (1984). While this is not strictly physically accurate (see, e.g., Combi 1996), the variation over the majority of the coma is relatively small. We use a temperature profile that varies with radial distance from the nucleus, having closely followed Combi's (1989) model (see Figure 1), and we can scale the initial gas temperature (at the surface) to alter our profile. These approximations make integration over time equivalent to calculating these values over increasing distances from the comet nucleus for a "shell" of gas expanding outward from the nucleus. (See, e.g., Bockelée-Morvan & Crovisier 1987, Combi 1996, Tenishev et al. 2008, etc., for more detailed and accurate treatments of coma temperature and velocity, parameterized over production rates, etc. For the present purpose of presenting our adaptation of CEP, the specifics of the coma integration model do not represent a limitation on our approach to radiative transfer.)

We ignore the photodestruction of CO in our coma model, due to its long lifetime (see Crovisier 1994). The lifetime is $>10^7$ s, and we are integrating out to 10^5 km with an expansion velocity of 0.8 km s⁻¹. (Note that others, e.g., Huebner et al. 1992 and Morgenthaler et al. 2011, find a shorter lifetime, but still $\gtrsim 4 \times 10^5$ s, or $\gtrsim 1.4 \times 10^5$ s, which is still large enough that it can be neglected in our modeling out to 10^5 km. Even for the smaller of these values, only in the outer coma, $\gtrsim 2.5 \times 10^4$ km, would the densities be reduced by $\gtrsim 10\%$. As we are primarily interested in optical depth effects in this study, the outer coma, where optical depths will be lower, is of less interest.)

The model can include coma morphology features as well, each modeled with its own coma integration using separate conditions. Such features, as seen in the Deep Impact and EPOXI encounters, are a main motivation for creating this model to better understand possible optical depth effects in the near-nucleus regions of the coma (see, e.g., Feaga et al. 2007; A'Hearn et al. 2011). After describing our method in Section 2, we present (in Section 3) some results demonstrating its use in better understanding possible optically thick spectra for the carbon monoxide 1-0 $(X^1\Sigma^+)$ band in spherically symmetric comae. These may be useful for ground-based (or space-based) observations of comets. In Section 4, we apply our CO model to actual spectra of comet Garradd, observed at 2 AU by the Deep Impact spacecraft. Forthcoming model results for CO₂, H₂O, and near-nucleus morphological features will follow (in other papers).

2. OUR METHOD: CEP ADAPTED FOR AN ASYMMETRIC SPHERICAL CASE

This section describes our adaption of the CEP radiative transfer technique to spherical cases in which the plane-parallel approximation is not appropriate, including most cometary problems. (Note that Yun et al. 2009 previously adapted CEP for *purely symmetric* spherical cases.) We have developed this model specifically for use in studying cometary comae, but it could be applied to many other astrophysical phenomena as well (planetary atmospheres, molecular clouds, etc.).

We derive expressions analogous to the relevant CEP06 equations, adapted from the plane-parallel situation to spherically symmetric cases. Then we include asymmetries of two different types: radiation from an outside source (here, the Sun) and non-uniform conditions due to morphology.

In brief, the CEP method (see CEP06) divides up a planeparallel "slab" into "zones" (each of which has uniform properties) and calculates the net radiative bracket ("p") that is multiplied by the Einstein A coefficient in the equations of statistical equilibrium (see Equation (1)) for each radiative transition for each zone. (Note that the "p" term effectively combines the "B" terms into the "A" term. See CEP06 for more details.) The innovation of CEP is that the net radiative brackets for each zone can accurately represent the contributions of all zones' emission and absorption to/from other zones (as opposed to "plain" Escape Probability, where a similar factor added to the statistical equilibrium equations is only a *local* approximation of a photon's likelihood of escaping the entire slab; see Bockelée-Morvan 1987; Zakharov et al. 2007; Litvak & Kuiper 1982). The statistical equilibrium equations for all zones, with the inclusion of the net radiative bracket, form a single non-linear matrix. This matrix can be solved using an algorithm for non-linear matrix solving such as Newton's method. We use functions from Numerical Recipes in C (see Press et al. 1992) for the Newton based matrix solver, as well as other calculations such as numerical integration. Further computational details can be found in the Appendix. This solution yields the fractional populations of molecular energy levels for each zone. From these, the flux emitted by the slab can be calculated. See CEP06 for more

2.1. Theoretical/Analytical Expressions for the Net Radiative Bracket

In CEP06 Equation (7), Elitzur & Asensio-Ramos derive a purely analytical expression for the net radiative bracket in a plane-parallel slab, based on the formal solution of the radiative transfer equation and the definition of the net radiative bracket:

$$p(\tau) = 1 - \frac{1}{2S(\tau)} \int_0^{\tau_t} S(t)dt \int_{-\infty}^{\infty} \Phi^2(x)dx$$
$$\times \int_0^1 e^{-|\tau-t|\Phi(x)/\mu} \frac{d\mu}{\mu}, \qquad (2)$$

where τ and *t* refer to optical depths for a specific wavenumber, with τ_t being the overall optical thickness of the slab, $S(\tau)$ or S(t) to the source function for a given line $(S_{\nu_{21}} = (A_{21}n_2/B_{12}n_1 - B_{21}n_2))$, $\Phi(x)$ is a dimensionless line profile, and $\mu = \cos \theta$, where θ is the angle of a given ray measured from the normal to the plane.

We use a spherical analog to this theoretical expression (i.e., as opposed to the discrete expression introduced later in CEP06 involving a number of "zones") for the net radiative bracket:

$$p(\tau(r,\theta,\phi)) = 1 - \int_{4\pi} \left[\frac{1}{2S(\tau(r,\theta,\phi,\Omega))} \times \int_{0}^{\tau(r,\theta,\phi,\Omega)} S(t(r,\theta,\phi,\Omega)) \times \int_{-\infty}^{\infty} \Phi^{2}(x) (e^{-|\tau(r,\theta,\phi,\Omega)-t(r,\theta,\phi,\Omega)|\Phi(x)}) dx dt \right] d\Omega, \quad (3)$$

where $p(\tau(r, \theta, \phi))$ refers to the net radiative bracket at any point labeled by the coordinates (r, θ, ϕ) in spherical coordinates with the origin at the center of some sphere of interest. (In our study, the sphere is centered on the comet nucleus; it could be the center of any spherical astronomical object for any given case.)

As in CEP06, $\Phi(x) = (\pi \Delta v_D)^{-1/2} e^{-x^2}$ is a dimensionless line profile, normalized so that $\int \Phi(x) dx = 1$, where $x = (v - v_0)/\Delta v_D$ is the dimensionless line shift from line center v_0 and Δv_D is the Doppler line width, $v_0/c(2kT/m)^{1/2}$. In the present work, we extend the CEP06 treatment of line profiles (which for the sake of presentation of a simple example used a $\Phi(x)$ that was the same throughout). We have included variations in line width (due to temperature) and Doppler shifts between different regions of the coma. The latter have been calculated for all three relevant aspects of the model with differing line-ofsight velocities: incident solar radiation, emergent flux along the observers' line of sight, and the calculation of the net radiative bracket between regions in the coma.

Both $\tau(r, \theta, \phi, d\Omega)$ and $t(r, \theta, \phi, d\Omega)$ refer to optical depths and $S(\tau(r, \theta, \phi, d\Omega))$ to the source function *as viewed from the coordinates* (r, θ, ϕ) along a "pencil" of solid angle $d\Omega$ (see Figure 2).

The optical depth along a "pencil" (or cone) of solid angle $d\Omega$ is, of course, highly dependent on the particular direction of a given solid-angle element $d\Omega$, i.e., dependent on θ', ϕ' , the direction of a vector centered on (r, θ, ϕ) pointing along the centerline of $d\Omega$ (see Figure 2).

2.2. Discrete Expressions for p

The above CEP06 expression for $p(\tau)$ (Equation (2)) is turned into a discrete expression by dividing the slab into multiple



Figure 2. Sphere showing a point (r, θ, ϕ) and two solid-angle elements $d\Omega_1$ and $d\Omega_2$. (Viewed from the -y direction.)

"zones" (labeled with indices i and j). This yields CEP06 Equation (14):

$$p^{i} = 1 - \frac{1}{2\tau^{i,i-1}S^{i}} \sum_{j=1}^{z} S^{j} \times \int_{\tau^{i-1}}^{\tau^{i}} d\tau \int_{\tau^{j-1}}^{\tau^{j}} dt$$
$$\times \int_{-\infty}^{\infty} \Phi^{2}(x) dx \int_{0}^{1} e^{-|\tau-t|\Phi(x)/\mu} \frac{d\mu}{\mu}.$$
 (4)

This expression for p can be calculated for each zone (and each wavenumber/frequency) and the resultant p values included in the equations of statistical equilibrium, which are then solved. (See also CEP06 Equations (32)–(36), and accompanying CEP06 text, for a more complete discussion.)

Similar to CEP06 Equation (14), for the purposes of our integration of a discretized p^i the sphere is divided into spherical shells (analogous to the plane-parallel zones of the original CEP) where *i* (or *j*) is a shell index (see Figure 3). The integration is broken down into a sum of integrals along different "cones" of solid angle (the aforementioned $d\Omega$'s). Note that although $d\Omega$ may seem somewhat conceptually analogous to $d\mu$ in the plane-parallel case, we cannot use the convenient exponential integrals as in the plane-parallel situation, but instead must integrate along each $d\Omega$ separately:

$$p^{i} = 1 - \int_{4\pi} \left[\frac{1}{2\tau^{i,i-1}(\Omega)S^{i}} \sum_{j=1}^{z} S^{j} \int_{\tau^{i-1}(\Omega)}^{\tau^{i}(\Omega)} d\tau \int_{\tau^{j-1}(\Omega)}^{\tau^{j}(\Omega)} dt \right. \\ \times \int_{-\infty}^{\infty} \Phi^{2}(x) dx (e^{-|\tau(\Omega) - t(\Omega)|\Phi(x)}) \left] d\Omega.$$
(5)

Here we have dropped the coordinate subscripts r, θ, ϕ for clarity/simplicity and use shell indices instead (where some shell *i* contains the point defined by r, θ, ϕ). Note that the "z" in the summation, the maximum number of shells along a given $d\Omega$, will be different for each $d\Omega$. For each "cone" of solid angle we will sum $S^{j}(\Omega)e^{-|\tau-t|}$ from "z" (the outermost shell) to i + 1, where i + 1 is the shell adjacent to shell *i*.



Figure 3. Example sphere showing division into four shells, i = 1...4, and solid angle $d\Omega_1$ for which z = 2 with indices j = 1, 2, as per Equation (5). (Viewed from the -y direction.)

2.3. Further Steps toward Implementation

In actual practice (i.e., computer implementation), the integration of the source function of $d\Omega$ over 4π steradians will also be done by a discrete summation.

Along any particular element of $d\Omega$ originating in shell *i*, this sum will be

$$\sum_{j=1}^{z} S^{j}(d\Omega) (1 - e^{-\tau^{j,j-1}(d\Omega)}) e^{-\tau^{j-1,i}(d\Omega)}$$
$$= \sum_{j=1}^{z} S^{j}(d\Omega) (1 - e^{-\tau^{j,j-1}(d\Omega)}) \prod_{j'=j-1}^{i} e^{-\tau^{j'}(d\Omega)}.$$
 (6)

Note that unlike the plane-parallel case, each $d\tau$ must be calculated explicitly from the geometry and local molecular energy level populations for each shell along the "pencil":

$$d\tau^{j}(d\Omega) = \alpha^{j}(d\Omega) \times ds^{j}(d\Omega), \tag{7}$$

where $\alpha^j(d\Omega)$ is the absorption coefficient in region *j* and $ds^j(d\Omega)$ is the distance through that region. Note that this distance may vary over the width of a given $d\Omega$, but we can either approximate using the centerline of $d\Omega$ or derive a θ' -dependent expression and calculate a proper integration to get a mean value over the region. (In our implementation we use the former option, for the sake of simplicity.)

This integration over solid angle is more tedious than in the plane-parallel case (which was able to use exponential integrals over a zone's $d\tau$) and more computationally costly, but straightforward enough to be feasible.

Turning this all into a fully discrete expression for p^i (for shell "*i*"), we get

$$p^{i} = 1 - \sum_{\omega=1}^{Z} \left[\frac{1}{2\tau_{\omega}^{i,i-1}S_{\omega}^{i}} \sum_{j=1}^{z} S_{\omega}^{j} \left(1 - e^{-(\alpha_{\omega}^{j} \times \Delta s_{\omega}^{j,j-1})}\right) \times \prod_{j'=j-1}^{i} e^{-(\alpha_{\omega}^{j'} \times \Delta s_{\omega}^{j',j'-1})} \times \Delta \Omega_{\omega} \right], \qquad (8)$$



Figure 4. 2D cross section of sphere on y = 0 plane, viewed from the -y direction, showing division into four shells, *with* superimposed cylinders along solar (\hat{z}) direction.



Figure 5. Two examples of different possible shapes of three-dimensional annuli formed by intersecting spheres and cylinders.

where Z is the maximum numbered spherical shell and all the quantities indicated by the subscript ω are dependent on a particular direction viewed from a given point (or shell *i*, in a spherically symmetric case).

2.4. Asymmetric Case: Incident Radiation

Our motivating interest in this study is comets' comae, which are *not* spherically symmetric cases.

To adapt CEP to this asymmetry, we divide each shell further into "regions." In the case of comets, one source of asymmetry is incident solar radiation coming from one direction (outside the outermost shell). Therefore, the natural way to further divide shells into regions is along lines parallel to the direction of solar radiation (i.e., the center-of-comet-to-center-of-Sun line, which we will arbitrarily label as the *z*-axis). Thus, we superimpose a set of co-axial cylinders (with radii equal to corresponding shell radii, for the sake of simplicity) on the shells to divide the coma into regions bounded by two cylinders and two spherical shells. (Note that some regions, specifically those along the z = 0plane perpendicular to the solar radiation, are only bounded by an inner cylinder and outer sphere. See Figures 4 and 5.)

These regions form annuli or rings of unusual, but easily envisioned, cross sections (see Figure 5).

Incident solar radiation is parallel to the z-axis (due to our choice of the z direction). Hence, each ray of sunlight travels along the axial direction of a specific cylinder. For each region, the solar radiation absorbed is calculated based on the relevant

optical depths along that direction (the $d\tau$'s) of those regions in the same cylinder that are closer to the Sun than the given region. This is similar to the case of external radiation described in CEP06 Appendix A, Equations (A3) and (A4), in which we simply set $\mu_0 = 1$, due to the above constraint of cylinders being co-axial with the incident solar radiation:

$$\bar{J}_e^i = J_e \frac{1}{\tau^{i,i-1}} \left[\gamma(\tau^i) - \gamma(\tau^{i-1}) \right],\tag{9}$$

where

$$\gamma(\tau) = \int_{-\infty}^{\infty} [1 - e^{-\tau \Phi(x)}] dx,$$

where J_e^i is the average over a region *i* of J_e^i , the contribution of external radiation, J_e , to the mean intensity of the region, which is to be included in the equations of statistical equilibrium (Equation (1)) by addition to the "B" term.

From a purely radiative standpoint, assuming that within each region there exists uniform density, temperature, and other physical conditions, the radiative excitation of molecules (hence the emission and absorption) in each region/annulus should be equal throughout the region. In our expanded CEP implementation, these regions are analogous to zones in the plane-parallel CEP. Each region's radiative effect or contribution to each other region, i.e., the net radiative bracket, must be calculated. Note that self-irradiation from around an annulus must also be taken into account, as well as irradiation from other regions. Once this calculation is done, the entire region will be equal with respect to radiative processes (i.e., there is symmetry around the z-axis).

2.5. Further Asymmetry: Coma Morphology

If models of distantly observed comets were all we needed, this might be sufficient. However, we are motivated by the desire to better understand *Deep Impact* and *EPOXI* spectral observations that have very high spatial resolution around the comets' nuclei (see, e.g., Feaga et al. 2007, 2011). Therefore, the above radiative treatment alone is insufficiently asymmetric to *fully* model a cometary coma, when coma morphology is included in the model. The inclusion of morphology undoes the aforementioned symmetry around the *z*-axis within each annulus/ region. These observations are one of the primary motives for this study, and therefore these morphological asymmetries must also be dealt with appropriately in this model.

To model morphological features, we use a cone shape superimposed over the aforementioned divisions into regions. (Other geometric shapes could also have been used. We chose to implement a cone due to its similarity in shape to many observed coma features.) A cone of arbitrary orientation and size with its vertex at the center of the sphere creates intersections with the above-described regions. Each of these is then added as a sub-region, which may have different properties from the surrounding (or subsumed/replaced) region.

Each sub-region can possess different initial conditions from the surrounding region. Thus, morphological features, which by their nature tend not to be axisymmetric around our z-axis, can be included in the model. It should be noted that these sub-regions are only included as necessary. Thus, for those annuli that *do* have constant axisymmetric conditions (i.e., no interesting morphological features impinging on them), we can save time and memory computationally by leaving them undivided, as they would have been originally.

2.6. Implementation: Our Algorithm Described

Given the above geometric divisions, we have implemented Asymmetric Spherical CEP as follows. For each region (or subregion, as applicable) we take representative population values from the coma integration and use these as the basis of an "initial guess." We then make an immediate improvement to the initial guess values by recalculating each region's populations (individually) taking into account the attenuation of incident solar radiation by intervening regions in the solar direction (as per Equation (9)). These recalculated populations are the values we then use as the initial guess (required by the implementation of Newton's method in Press et al. 1992) for CEP calculations. Based on these populations, we calculate the necessary source functions, delta-taus, and net radiative brackets, "p," as above, for each wavenumber (or line, transition, etc.). Following the above discretized Equation (8) for each region, which in this context we will call the "recipient" region, we iterate over all other regions to calculate their contribution to the recipient's p. Each other region's contribution is essentially its own source function attenuated over the optical depth of all intervening regions along the line of sight between itself and the recipient region, integrated over (or, to simplify, multiplied by) the solid angle subtended by one region from the other. This is then divided by the recipient region's source function and optical depth (along the given line of sight).

To implement this in a practical algorithm of manageable complexity, we make several simplifying approximations.

Due to the z-axis symmetry that exists (before adding subregions), we can *partially* simplify to a two-dimensional (2D) diagram in which a region is represented by the cross section of the annulus in the (arbitrarily chosen) y = 0 plane. We calculate a region's "centroid," i.e., the centroid of its 2D projected area in this plane that (in our approximation) corresponds to a point (r, θ, ϕ) in spherical coordinates.

For (cone-shaped) sub-regions, which in general do not have their centerline on the X-Z plane, we must use a different centroid. We use the midpoint along the cone's centerline (within region boundaries).

We also choose a series of points distributed evenly along circles parallel to the X-Y plane around each region, which will be the "starting points" for calculation of lines of sight (which will terminate at the centroids). These are chosen by rotating a region's centroid around the *z*-axis by multiples of some angle that depends on the size (radius) of the region. The choice of angle is such that the larger a region's size, the more starting points it will have, and thus the region will be divided into more elements of solid angle.

We use the line of sight between the "centroids" of regions and this series of starting points to calculate the contributions of every other region (or the region to itself) to a given recipient region's p. We calculate the optical depth of each intervening region, along the line of sight, based on the molecular population levels of the intervening regions (see Figure 6). These "integration lines" encapsulate the main part (within the square brackets in Equation (8)) of the calculation of p.

We approximate the solid angle subtended by the integration lines from another region's centroid by integrating $d\Omega = d\phi$ sin $\theta d\theta$ from zero up to the mean value of the angles between the starting point of that region, the centroid of the recipient region, and the multiple "corners" of that region around the

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Figure 6. Two-dimensional view from above (i.e., the +*z* direction) of examples of integration lines in the X-Y plane. Four lines originating in the i = 1 region and ending at the centroid of the i = 2 region are shown (red in the online version), with corresponding division of the i = 1 circle (shown by dashed gray lines). Eight lines originating in the i = 4 region and ending at the centroid of the i = 3 region are shown (blue in the online version), with corresponding division of the i = 4 region and ending at the centroid of the i = 3 region are shown (blue in the online version), with corresponding division of the i = 4 annulus (also shown by dashed gray lines). One example of a corresponding $d\Omega$ is also shown with dot-dashed lines (green in the online version). Note that this 2D diagram only shows horizontal cross sections of regions, and so regions and shells/annuli are essentially indistinguishable in this diagram.

(A color version of this figure is available in the online journal.)



Figure 7. Example illustrating calculation of mean angle. Lines originating from an angular slice of a region's "corners" and terminating at another region's centroid are shown in black. The line between the centroid of the "recipient" region and a "start point" of the other region (the largest dot) corresponds to the relevant integration line (and is shown in red in the online version). The integration line and each of the other eight lines define the angles that are averaged together to get the mean angle θ_{mean} used to calculate the solid angle subtended by one region as viewed from the other's centroid. Note that not all regions will have eight "corner points."

(A color version of this figure is available in the online journal.)

starting point (see Figure 7). Effectively, this gives a solid angle between regions of $2\pi(1 - \cos \theta_{\text{mean}})$.

Note that due to these approximations, the sum of solid angles over all integration lines between a region and all regions in a given shell exterior to the region is *not* necessarily constrained to exactly equal 4π , as it should be in reality. Therefore, in calculating a "p" value, we sum the solid angles involved and



Figure 8. As per Figure 4 above, with observer plane also shown, aligned perpendicular to the X-axis.

(A color version of this figure is available in the online journal.)

average over that sum instead of 4π steradians (as Equations (3) and (5) dictate we should do).

In the limit of arbitrarily small (and numerous) regions, these approximations *would* approach a physical situation of arbitrarily precise accuracy. Thus, we maintain the "exactness" of the CEP method.

Unlike the plane-parallel situation, the flux exiting the surface of the coma (or other sphere of interest) is not simply a single value (per wavenumber) that has been integrated over angle. In the spherical situation, the resultant intensities form a 2D mapping (in a plane perpendicular to the observer's line of sight; see Figure 8).

In our implementation, this plane is specified by rotation angles, θ , ϕ , and ψ with the comet's center at the origin, and is assumed to be at a distance $\ge R_{\text{coma}}$, the maximum radius of the coma. We can also specify the density of and interval between points on this plane for which the output intensities will be calculated. Each point in this planar mapping shows the intensity (or surface brightness) integrated along a specific line of sight, perpendicular to the plane, through the coma from one side to the other (again, for each wavenumber):

$$I_{\text{surf}} = \sum_{i=1}^{z} \left(S_i \Delta \nu_i \left(1 - e^{-\tau^i} \right) \prod_{j=i-1}^{j=1} e^{-\tau^j} \right), \quad (10)$$

where S_i is the source function of a region i, Δv_i is the line width of wavenumber/frequency v in region i, and τ^i , or τ^j , represents the optical depth of wavenumber v in region i or j along the relevant line of sight. Indices i and j run from 1 to z, where z equals the number of regions along a given line of sight.

Thus, the spherical CEP algorithm produces results that could be described as a four-dimensional data "hypercube": for each point in the above 2D mapping, there is a complete (2D flux versus wavenumber) spectrum. These data can then be presented

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 Table 1

 Model Input Parameters for Models of Theoretical Example Comets for CO

| Parameters | Values | |
|--------------------------------------|---|--|
| Mean nucleus radius | 3 km | |
| T _{surface} | 200 K | |
| Expansion speed V_{exp} | 0.8 km s^{-1} | |
| Qco | $10^{26}, 10^{27}, 10^{28} \text{ s}^{-1}$ | |
| Band center wavenumber | 2149 cm^{-1} | |
| Band center Einstein A | 33 s^{-1} | |
| Highest rot. level, J_{max} | 20 | |
| Solar flux | $2.5 \times 10^{13} \text{ photons cm}^{-2} \text{ s}^{-1} (\text{cm}^{-1})^{-1}$ | |
| $\sigma_{ m rot}$ | $1.32 \times 10^{-14} \text{ cm}^2$ | |
| | | |

| Table 2 | | | |
|---|--|--|--|
| Reproduction of Chin & Weaver's Table of CO-H2O Collision | | | |
| Cross-section Information | | | |

| $\Delta J = J_{\rm upper} - J_{\rm lower}$ | Fraction of Total De-excitation | | |
|--|---------------------------------|--|--|
| 1 | 0.34 | | |
| 2 | 0.25 | | |
| 3 | 0.20 | | |
| 4 | 0.10 | | |
| 5 | 0.07 | | |
| 6 | 0.05 | | |
| >6 | 0 | | |

Notes. Total cross section is always $\sigma_{rot} = 1.32 \times 10^{-14} \text{ cm}^2$. Excitation is derived from de-excitation using detailed balance.

in multiple formats. Several forms of data presentation for simulating observations are described in the following section.

This is also precisely the output needed to compare with the *Deep Impact* and *EPOXI* observations that have been displayed as 2D brightness maps for specific wavelengths or bands.

3. SOME PRELIMINARY RESULTS: OBSERVABLES FOR DISTANT COMETS

We present here examples of model results for three different production rates of carbon monoxide that could be potentially useful for distant (e.g., ground-based or orbital telescope) observers of comets. These are modeled using a spherical coma, without any morphological features but including optical depth effects both with respect to incident solar radiation within the coma and with respect to emergent "observed" radiation.

The output data from the CEP model can be presented in various ways. Here we show an example of a band total brightness map (analogous to Feaga et al. 2007, but for the entire coma), radial profiles of brightness, column density, and *g*-factors for various azimuthal angles. (These could also be done for individual spectral lines, but in the interests of space and avoiding complexity we have not presented such results here.) We also present spectra integrated over different "aperture" sizes. The band total brightness is more likely to be similar to actual observations, but high-resolution spectra are possible, even from ground-based telescopes (see, e.g., DiSanti et al. 1999, 2001), in particular for comets close to Earth, which might more closely resemble the latter form of model results.

We also demonstrate the potential usefulness to observers of the ratio of the total brightness of the P branch to that of the R branch of CO to determine whether observations include significant optical depth effects. This may be measurable even with relatively poor spectral resolution. CO 1-0 Band Tot. Brightness Map, Q=10²⁸s⁻¹ (Phase angle=90°)



Figure 9. Example of a band total brightness map for the CO 1–0 band, for the inner ± 600 km near the nucleus of a theoretical comet with $Q_{\rm CO} = 10^{28}$ s⁻¹, viewed from phase angle = 90°. Overlaid radial lines indicate the orientation of azimuthal angles in radial profiles below. The sunward direction is up, i.e., azimuthal angle = 0°. Note that within the ± 600 km field of view, the brightness never reaches zero (even where it appears to be totally dark). This image is in color in the online version of the article, and the colors of the azimuthal angles correspond to those in subsequent radial profiles.

(A color version of this figure is available in the online journal.)

Many of the model "input values" (see Table 1) have been chosen so as to facilitate comparisons (of our optically thin cases) with other earlier models. Model parameters that are the same for all the following examples are: Solar distance = 1 AU. Solar flux (over the CO band) is 2.5×10^{13} photons cm⁻² s⁻¹ (cm⁻¹)⁻¹, as per Labs & Neckel (1968) (and as used by Chin & Weaver 1984 and Weaver & Mumma 1984). Note that the model/code is able to read a (solar) flux input file and thus could use a more detailed and accurate solar spectrum (e.g., including Fraunhofer lines). The simplification of using a constant incident solar flux does not represent a limitation of the model. Also note that for comet Garradd, which we have modeled here (see Section 4), the heliocentric velocity at the time of observations was 14.5 km s⁻¹, well above a value likely to cause significant Swings effects (e.g., $\pm 5 \text{ km s}^{-1}$; see Kim 1996). Gas expansion speed is a constant 0.8 km s^{-1} , and the initial gas temperature at the surface is 200 K. $Q_{\rm H_2O} = 10 \times Q_{\rm CO}$, as in Chin & Weaver (1984). As mentioned above, the radial temperature profile closely follows Combi's (1989) model (see Figure 1) but scaled to the initial gas temperature at the surface, T_{surface} .

The coefficients for CO–H₂O collisions (assumed to be the dominant source of collisional excitation) are as per Chin & Weaver (1984): only rotational excitation and de-excitation are considered. (Vibrational cross sections are about five orders of magnitude smaller. See Weaver & Mumma 1984, Table 2.) $C = n_{\rm H2O} \sigma \bar{v}$, where \bar{v} is the average relative speed of the molecules (cm s⁻¹), $n_{\rm H_2O}$ is the number density of H₂O (cm⁻³), and σ is the collisional cross section of a given transition of CO (cm²). The last value is based on a total cross section of $\sigma_{\rm tot} = 1.32 \times 10^{-14}$ cm², which is apportioned between $\Delta J's$ up to 6 as per Chin & Weaver's Table 1, which we reproduce here in our Table 2.

3.1. Brightness Maps

We present here one example of a brightness map of a modeled coma (see Figure 9). This format of output presentation is most similar to the radiance maps of Feaga et al. (2007) and A'Hearn et al. (2011). For a spherical coma with no morphological features, it is rather uninteresting. It is nevertheless included here as a demonstration and used to illustrate the azimuthal angles of the radial profiles presented below with the addition of overlaid lines. Note that for the $Q_{\rm CO} = 10^{28} \text{ s}^{-1}$ case, there is some difference in brightness noticeable to the eye between the sunward side (azimuthal angles nearer to zero) and the anti-sunward side, especially in the near-nucleus portion of the image. This is due to the optical depth along the solar direction reducing the excitation and emission from one side of the coma to the other.

3.2. Radial Profiles: Brightness, Column Density, and g-factors

Abundances of cometary species are frequently calculated from observed fluxes using fluorescence efficiencies, or *g*-factors. In an optically thin case, the brightness of a given line or band is proportional to the column density of the relevant molecule. In such cases, $F_{\text{band}} = g_{\text{band}} \times N$ and $g_{\text{band}} = \sum_{\text{band}} A_u \times n_u$, where F_{band} is the band total flux (or brightness), g_{band} the band *g*-factor, *N* the total column density, A_u the Einstein *A* coefficient for the relevant transition originating in upper level "*u*," and n_u the column density of the population of a specific upper level "*u*" (which in our model is numerically approximated as the sum over all regions along a line of sight of the fractional population of level "*u*" times each region's column density).

However, large optical depths will spoil this simple linear relation between column density and brightness. With radiative transfer modeling, it is possible to get a calculated *g*-factor ($g_{\text{band}} = \sum_{\text{band}} A_u \times n_u$) from the model and the "effective *g*-factor," $g_{\text{eff}} = F_{\text{band}}/N$, which is the actual ratio of brightness to column density.

In Figures 10, 11, and 12 we present all these values together as radial profiles, for theoretical comets of three different production rates, $Q_{\rm CO} = 10^{26}$, 10^{27} , and 10^{28} s⁻¹. (All are observed at 1 AU, at a phase angle of 90° and multiple azimuthal angles. In all cases $Q_{\rm H_2O} = 10 \times Q_{\rm CO}$.)

In our results, we typically see that g_{eff} does tend toward the calculated g-factor values at larger impact parameters, where optical depth effects are negligible, as would be expected. (The actual numerical values of the "asymptotic" band g-factors produced by our model, 2.4×10^{-4} s⁻¹ per molecule for CO at 1 AU, also agree well with other published values, such as those calculated by Chin & Weaver 1984; Crovisier & Le Bourlot 1983; and Weaver & Mumma 1984.) The actual radii at which this convergence occurs depend primarily on the production rate of a comet. We can use the distance at which $g_{\rm eff} = 0.9 g_{\rm thin}$ as a very rough measure of the point where a coma can be considered to transition from optically thick to thin. For the "thin" and "intermediate" coma models $(Q_{\rm CO} = 10^{26}$ and $Q_{\rm CO} = 10^{27} \, {\rm s}^{-1})$ the convergence is fairly close to the nucleus, within \sim 100–200 km. However, for the "thick" model $(Q_{\rm CO} = 10^{28} \text{ s}^{-1})$ with its high production rate, the "optically thick regime" can extend as far as $O(10^3)$ km, which can be spatially resolved even in some remote observations. Note that at radial distances very near the nucleus, worrying about optical depth effects may be relevant even for lower production rates.

3.3. Radial Profiles: Phase and Azimuthal Angular Variations

Another optical depth effect is variation of brightness (and corresponding *g*-factor) with varying angles, both phase angle (of observer) and azimuthal angle within any given observation.

CO 1−O Band Tot. Hypoth Q_{co}= 1×10²⁶s⁻¹: Brightness, Col. Density & Ratio vs. R (Phase angle=90°, Multiple Azimuthal angles)



Figure 10. For $Q_{\rm CO} = 10^{26} \text{ s}^{-1}$. Upper frame: radial profile of band total brightness vs. *R* (impact parameter) for phase angle = 90° and for multiple azimuthal angles. Profiles of azimuthal angles (indicated by color coding in the online version) show no variation for this case and overlap, appearing indistinguishable. Column density is included as the bold solid line (red in the online version) using a different *y*-axis scale. Lower frame: *g*-factors. Both the calculated *g*-factor (the higher group of lines) and *g*_{eff}, the observed brightness over column density, are plotted with matching styles (colors in the online version) for each azimuthal angle (which also match those in the upper frame). Profiles for 0°, $\pm 45^{\circ}$, and 90° overlap each other almost entirely. (A color version of this figure is available in the online journal.)

The radial profiles in Figures 10-12 demonstrate the azimuthal variation for a single phase (observing) angle. It may seem somewhat surprising and counterintuitive that the radial profile lines in the sunward direction are not the brightest (nor those closer to sunward on either side). However, when velocities and Doppler shifts are accounted for, this is readily explained. Along the sunward (or anti-sunward) direction there is no change in the sunward component of the expansion velocity, and thus no relative Doppler shifting of the line-center frequencies, all along that direction. This causes greater effective optical depths and less solar excitation in that direction. Conversely, the profiles of directions perpendicular to sunward show greater excitation. Even for the only moderately thick case of $Q_{\rm CO} = 10^{27} \, {\rm s}^{-1}$ for radii $\leq 100 \, {\rm km}$, there is a difference of as much as \sim 5%–10% between sunward and anti-sunward directions. The effect is even more pronounced (as much as $\sim 20\% - 30\%$) for the thicker case of $Q_{CO} = 10^{28} \text{ s}^{-1}$.

In Figures 12–16, we present profiles of brightness (and column density) for model results observed from different phase angles, ranging from 0° to 180° , for the optically thicker case of $Q_{\rm CO} = 10^{28} \text{ s}^{-1}$. Each plot includes multiple azimuthal angles, which would all be visible simultaneously in a wide-field observation (i.e., including the entire coma) from each



Figure 11. For $Q_{\rm CO} = 10^{27} \, {\rm s}^{-1}$. Radial profiles of brightness, column density, and *g*-factors as per Figure 10. Profiles of azimuthal angles (indicated by color coding in the online version) for 0° , $\pm 45^{\circ}$, and 90° overlap each other almost entirely, and other brightness profiles are almost indistinguishable. Lower frame: profiles of azimuthal angles 0° , $\pm 45^{\circ}$, and 90° overlap each other almost entirely and are almost indistinguishable. ("Jaggedness" of the profiles is due to the division into discrete regions in the model.)

given phase angle. (The above plot for 90° phase angle for $Q_{\rm CO} = 10^{28} \, {\rm s}^{-1}$, Figure 12, should be considered part of this series as well.)

Observations with a slit spectrometer with sufficient spatial resolution (see, e.g., DiSanti et al. 1999) might observe along one specific azimuthal angle and thus see possible variations along the slit with sufficiently high spatial resolution.

The most obvious effect seen at a glance in these figures is the spread among azimuthal angles for a given phase angle. As would be expected, the 0° and 180° phase angles (sunward and anti-sunward) have no real azimuthal variation. From phase angle 45° to 90° to 135° there is a progression: the azimuthal lines get spread out farther from each other, as well as noticeably dropping in brightness for those lines farther from the sunward side.

With respect to total brightness, the phase angles 0° , 45° , 90° , and 135° produce roughly equal peak brightness for their *strongest* azimuthal profiles (the more sunward directions, at the nucleus grazing radius) of about $\sim 3 \times 10^{12}$ photons s⁻¹ cm² sr⁻¹. Most significantly, for the 180° phase angle, the peak values are about $\sim 2 \times 10^{12}$ – significantly less bright than at other phase angles.

With respect to "effective" (or "observed") *g*-factors, the minimum values in the most optically thick regions (again, at the nucleus-grazing radii) also show a trend from sunward to anti-



Figure 12. For $Q_{\rm CO} = 10^{28} \, {\rm s}^{-1}$. Radial profiles of brightness, column density, and *g*-factors as per Figure 10. Profiles of azimuthal angles (indicated by color coding in the online version) for 0° , $\pm 45^{\circ}$, and 90° overlap each other almost entirely.

(A color version of this figure is available in the online journal.)

sunward. For the 0° through 135° phase angles, the minimum values of the ratio of the band total flux over the column density are roughly 3×10^{-5} photons s⁻¹ molecule⁻¹, while for 180° the value decreases to a minimum of about 2×10^{-5} . This trend is due to a combination of two optical depth effects. The first is attenuation of incident solar light from the sunward to antisunward sides of the coma, leading to less fluorescent pumping, and thus less emission, by the anti-sunward direction. Second, whatever emission there is more likely to "escape" the coma along lines of sight along the azimuthal angles closer to where it is emitted, experiencing less total optical depth on its path out of the coma. Thus, the already greater emission of the sunward regions is also more likely to be observed along azimuthal directions closer to sunward.

However, the similarly located values for "actual" calculated *g*-factors do *not* follow a similar simple monotonic trend. The greatest values for a given phase angle rise from 0° through 45° and peak for phase angle 90°. From 90° through 135° down to 180° they fall through the same values, creating a symmetric peak around 90°. This symmetrical and non-monotonic pattern of the calculated values is less intuitive than the trend of g_{eff} over angles in the same cases. However, it is clearly understood in light of the fact that these values are based only on the actual population distributions in different regions and do *not* include optical depth effects on the *emergent* radiation. Thus, observing from phase angles 0° and 180° are sampling exactly the same lines of sight and regions' populations, including the





Figure 13. For phase angle = 0° , $Q_{CO} = 10^{28}$ s⁻¹. Radial profiles of brightness, column density, and *g*-factors as per Figure 12. Profiles of azimuthal angles (indicated by color coding in the online version) show no variation for this case (as should be expected) and overlap, appearing indistinguishable. (A color version of this figure is available in the online journal.)

least illuminated parts (i.e., least excited populations) of the anti-sunward side of the coma. The same is essentially true for 45° and 135° (due to symmetry around the *z*-axis), but they do not sample the darkest parts of the anti-sunward directions (and the differences in populations are less between outermost regions on the sunward side among azimuthal angles between ± 45 —they are all experiencing direct solar illumination). For 90° the higher azimuthal profiles are sampling from more excited and higher emission populations than the profiles with lower values, and consistently so all the way along their lines of sight (which is not true for 45° and 135°). Thus, the more sunward lines for 90° are the brightest seen, and the anti-sunward values fall between values of the 0° or 180° and the 45° or 135° lines.

Finally, the profiles for $Q_{\rm CO} = 10^{28} \text{ s}^{-1}$ have a deviation from linear slopes in their brightness in the vicinity of ~100 ~1000 km, most easily visible for the 180° plot, but also present for the other phase angles (and growing in size from 0° up to 180°). This is mostly due to the temperature profile reaching its minimal values at these radii in conjunction with the higher density of the $Q_{\rm CO} = 10^{28} \text{ s}^{-1}$ case. The higher density leads to this still being a collisionally dominated regime, and the low temperatures lead to the lowest population levels being most highly populated. These levels also have the highest Einstein A values, thus leading to a higher overall number of photons emitted for the same number of molecules. The effect is greatest for the 180° view due to a cumulative effect—the lines of sight all sample the most dense and cold regions at



Figure 14. For phase angle = 45° , $Q_{\rm CO} = 10^{28}$ s⁻¹. Radial profiles of brightness, column density, and *g*-factors as per Figure 12. Profiles of azimuthal angles (indicated by color coding in the online version) are slightly displaced for viewing purposes.

(A color version of this figure is available in the online journal.)

these radii. The same extreme effect is not seen for the 0° phase angle due to the overall greater fluorescent excitation of the sunward regions dominating it. (Note that the difference in total brightness between the two azimuthal angles at these radii is about a factor of two.)

3.4. Aperture-averaged Spectra

If one is observing with high spectral resolution but low spatial resolution, the spectra observed will be the sum of as much of the coma as fills the field of view. To model this, we have simulated "aperture-averaged" spectra, where the "aperture" controls the area of the coma sampled. Our apertures are square boxes and are all centered exactly on the center of the comet, and sample a nucleus-centered area equal to the square of the "aperture size" over which we average the brightness. We present a series of apertures from 2×10^1 km (very near the nucleus) through 2×10^5 km (the whole coma) for each of the three production rates. See Figures 17–19. (All these example spectra are modeled at a heliocentric distance of 1 AU and phase angle 90° . $Q_{H_2O} = 10 \times Q_{CO}$, as in Chin & Weaver 1984.)

Band shape for apertures including the outer coma (approximately $10^4 < R_{ap} < 10^5$ km) does not change significantly for different production rates. The total brightness for this regime increases approximately in linear proportion to production rate. This is due to spectra with such large aperture sizes being dominated by the fluorescence-dominated optically thin outer coma, with optical depth effects playing a minimal role (but not



Figure 15. For phase angle = 135° , $Q_{\rm CO} = 10^{28} \, {\rm s}^{-1}$. Radial profiles of brightness, column density, and *g*-factors as per Figure 12. Profiles of azimuthal angles (indicated by color coding in the online version) are slightly displaced for viewing purposes.

entirely non-existent: note the small, $\leq 3\%$, reduction in *g*-factor for the highest production rate model for $R_{\rm ap} = 2 \times 10^4$ km).

In the inner coma, however, optical depth effects can be very striking. The "thickest" spectra (for higher production rates and smaller $R_{\rm ap}$) have remarkably altered band shapes from the optically thin spectra.

First, however, a word about changes that are *not* specifically caused by optical depth effects. It is clear that there is much variation, even within a given production rate, from large to small aperture sizes. Not all of this is due to optical depth effects. Even in our optically thin case, the band shape changes noticeably in breadth. This occurs primarily due to the temperature profile. We have used a fairly simplified profile, which can be scaled to a surface temperature parameter but does not vary much otherwise between different model cases. This provides a straightforward "control" for this aspect of spectral change with aperture size.

In the innermost coma near the nucleus, the temperature is quite warm ($\sim 100-200$ K), which leads to a broader band in the 10 km spectrum. The coma gas cools to a minimum (~ 20 K) around 100–200 km out from the nucleus, which produces a much narrowed band. Since the Einstein A coefficient for the lowest J lines is higher than for the lines in the "wings" of the band, the cold temperature also increases the g-factor, even in optically thick regions. At larger radii, the temperature rises again, but becomes less significant since the coma gets less dense and tends toward fluorescent equilibrium. Between these



Figure 16. For phase angle = 180° , $Q_{\rm CO} = 10^{28}$ s⁻¹. Radial profiles of brightness, column density, and *g*-factors as per Figure 12. Profiles of azimuthal angles (indicated by color coding in the online version) show no variation for this case (as should be expected) and overlap, appearing indistinguishable. (A color version of this figure is available in the online journal.)

regimes, in a "transition region," there are still optical depth effects, which can be more easily isolated as *g*-factors are less temperature controlled.

Temperature is also a factor in determining Doppler broadening and line width, which is proportional to $T^{1/2}$, so the ratios between line widths for the coldest and the warmest regions of the coma are about 2–3, for a given wavenumber. This may lead to temperature playing a significant role in the optical thickness of the coma to incident solar radiation.

Temperature effects notwithstanding, the spectra from the denser near-nucleus regions of a coma show optical depth effects in several aspects. In addition to the total brightness no longer increasing linearly with production rate (and a corresponding reduction of g-factors), energy is also dramatically shifted between lines within the band.

The notable shifting of flux from *R* branch to *P* branch (evident in many of the thicker spectra) and shifting to lower wavenumbers in both branches (as is most evident in the $R_{\rm ap} = 20-200$ km spectra for $Q = 10^{28}$ s⁻¹) are very noticeable optical depth effects. (See Sahai & Wannier 1985 for an analytical discussion of similar effects.)

This effect appears due to the branching ratio of a given pair of *P*- and *R*-branch lines originating in the same upper level ((J' + 1)/J') for the pair of lines from upper level J', which generally (slightly) favors emission in the *P*-branch line. In optically thick cases, repeated absorption and emission of photons lead to a cumulative effect that favors the *P* branch over the *R* branch much more than in optically thin conditions (where it is probable that any emitted photon will not be re-absorbed before escaping the coma). See Figure 20.

Similarly, flux is "pushed" outward in the branches, and more so in the P branch due to combination with the above effect. This is due to the lines closer to the center of the band becoming optically thick before those in the wings (both due to their higher Einstein coefficients and generally being more populated). Flux initially emitted in lines that are optically thick will through repeated absorption and emission be forced out into lines that are less thick.

3.5. The P/R Ratio: a Useful Heuristic of Optical Depth

As seen in Figures 17–19, the *P*-branch total brightness and the *R*-branch total brightness vary with respect to each other over different optical depths (as well as other factors, such as temperature distribution). The ratio of the sums of P/R branches' brightnesses can be useful to alert an observer (or anyone analyzing observations) that they must in a given case beware of, and if possible account for, optical depth effects.

This alone would not be sufficient, as temperatures along a given line of sight are also a significant factor in controlling the P/R ratio, in the collisionally dominated inner coma. Colder population distributions will emit more in the lower lines (in both branches) for which the ratio of P/R for each pair of lines originating in the same upper state is greater. Also, the values of τ and $d\tau$ in Equations (2)–(10) will effectively vary inversely with line width, other factors being equal.

Use of a model like ours can show where the P/R ratio is large due to temperature and where (its excess beyond that value is) due to optical depth. In our optically thin, $Q_{\rm CO} = 10^{26} \,{\rm s}^{-1}$, model the P/R ratio does not exceed ~1.4, even for aperture sizes dominated by the coldest portion of the coma. (Note, however, that this is an aperture-*averaged* value. In Figure 21 below, the peak value is slightly higher, ~1.5.) However, the ratio for corresponding aperture sizes in the $Q_{\rm CO} = 10^{27} \,{\rm s}^{-1}$ and $Q_{\rm CO} = 10^{28} \,{\rm s}^{-1}$ cases is ~1.6 and ~1.9, respectively. Furthermore, in the thickest case modeled, even the spectrum with aperture size of 2000 km has a ratio of ~1.4. Note that in all cases the 2 × 10⁵ km aperture, which is dominated by the outer coma in fluorescent equilibrium, has a ratio of ~1.4–1.5 is a warning sign of optical depth effects involved.

3.6. Further Discussion

While it would be ideal to be able to derive a simple correction factor from the P/R ratio in such cases, alas, it is not exactly possible. However, a rough estimate of the degree of optical depth effects can be derived.

To do so, we create radial profiles of the P/R ratio, for both the observed emergent flux/brightness and the calculated value based on underlying populations without attenuation of emergent light, as shown in Figures 21, 22, and 23. By crossreferencing the observed P/R ratio for a given radial distance with the corresponding g-factor in Figures 10, 11, and 12, one can ascertain the "real" g-factor to use to calculate a correct column density from the observed flux.

This heuristic is, of course, limited in use to the carbon monoxide $X^1\Sigma^+$ band. Other spectra with *P* and *R* branches will have their own ratios, which can be derived by similar modeling. More complicated spectra may also, but such ratios would be more complicated to find than for cases with a simple two-branch structure.

4. MODELING RESULTS FOR COMET C/2009 P1 GARRADD: CO

Comet C/2009 P1 Garradd (hereafter just "Garradd") was observed by the *Deep Impact* spacecraft with both the mediumresolution instruments (MRI) and high-resolution instruments (HRI) when the comet was at a heliocentric distance of 2 AU post-perihelion.

All three of the volatile species we have modeled were observed simultaneously (see Figures 27 and 29). For further details of the Garradd observations and the corresponding modeling see, respectively, Feaga et al. (2014) and our forthcoming paper (A. M. Gersch & M. F. A'Hearn, in preparation), which will provide for CO_2 and H_2O a similar treatment to that which we present here for CO.

The H₂O ν_3 1–0 band is visible around 2.6–2.8 μ m, the CO₂ ν_3 1–0 band around 4.2–4.4 μ m, and the CO 1–0 band around 4.6–4.7 μ m (with two peaks visible for CO).

These observations provide an excellent test case for our model. Unlike the Tempel 1 and Hartley 2 observations, the CO band is very clearly detected in the spectra, and the observed spectra are from large apertures similar to the model results presented above (see Section 3.4). Furthermore, since there was minimal observational detail showing coma morphology (however, see Feaga et al. 2014 and T. L. Farnham et al. 2014, in preparation), this seemed an appropriate case in which to apply a spherically symmetric coma model. In keeping with the presentation above, we will concentrate on the carbon monoxide spectra in this paper.

4.1. Garradd DI HRI Observations

The DI-HRI observations of Garradd had sufficient signal-tonoise ratio (S/N) to detect the coma signal above the background and extract spectra from the data in a 5 \times 9 pixel aperture, corresponding to 21,050 \times 18,945 km² aperture, centered on the unresolved nucleus. (Note that the pixels are rectangular, not square.) Smaller apertures of 1 pixel and 3 \times 5 pixels, corresponding to apertures of 4210 \times 2105 km² and 12,630 \times 10,525 km², respectively, were also extracted from the data. The S/N for the CO band is \sim 3 in the largest aperture and as low as \sim 2 in the smallest. Thus, noise in the spectra (see Figures 27–29) is significant.

The *P* and *R* branches in the initial HRI Garradd CO spectra seemed to be somewhat but not very clearly distinguishable in some of the spectra. (See Figures 27–29.) For some aperture sizes the most obvious features could possibly be noise. (e.g., The single pixel wide "peaks" on the edges of the CO band's wavelengths.) However, the peak in the *P* branch at around 4.65 $\sim 4.675 \,\mu$ m is visible although it is a very narrow one and very close to the band center.

Comparison with our theoretical models implies that the observations are dominated by cold and collisionally dominated regions of the coma.

In addition to considerations of temperature, the large P/R branch ratio of Garradd CO fluxes also indicated that some optical thickness was involved (as per Figure 19 above). The peak of the *P* branch is much greater than that of the *R* branch (in those Garradd spectra where the *R*-branch peak can be distinguished).

The smallest aperture Garradd spectrum appears qualitatively similar in band shape and branch ratio to our hypothetical 200 km aperture CO spectrum for $Q = 10^{28} \text{ s}^{-1}$ (see Figure 19(c)) and the largest aperture spectrum somewhere



Figure 17. Aperture-integrated spectra for $Q_{\rm CO} = 10^{26} \, {\rm s}^{-1}$. Left side y-axis is aperture-averaged brightness. Right y-axis is effective (line) g-factor (brightness/column density). Totals are indicated on each graph.



Figure 18. Aperture-integrated spectra for $Q_{\rm CO} = 10^{27} \, {\rm s}^{-1}$. Left side y-axis is aperture-averaged brightness. Right y-axis is effective (line) g-factor (brightness/column density). Totals are indicated on each graph.



Figure 19. Aperture-integrated spectra for $Q_{\rm CO} = 10^{28} \, {\rm s}^{-1}$. Left side y-axis is aperture-averaged brightness. Right y-axis is effective (line) g-factor (brightness/column density). Totals are indicated on each graph.





Figure 20. Ratio of a sampling of individual pairs of *P*-branch/*R*-branch lines sharing a common upper J' level. Brightness vs. *R* (impact parameter) for the $Q = 10^{28} \text{ s}^{-1}$ case. (The lower *Q* models' corresponding profiles are essentially flat.) The asymptotic values are essentially the ratio of (J' + 1)/J'. (The small deviation from the exact ratio of (J' + 1)/J' is due to the ratio of the cube of wavenumbers in the Einstein *A* coefficient calculation in addition to the (J' + 1)/J' ratio.) Phase angle = 90° and for sunward and anti-sunward azimuthal angles. (Ratio profiles are indicated by color coding in the online version.)



Figure 21. For $Q_{\rm CO} = 10^{26} \, {\rm s}^{-1}$. Ratio of *P*-branch vs. *R*-branch total brightness vs. *R* (impact parameter) for phase angle = 90° and for multiple azimuthal angles. Profiles of azimuthal angles show negligible variation for this case and overlap, appearing indistinguishable. (Profiles are indicated by color coding in the online version.) "Sawtoothed" appearance of the plot is due to the division into discrete regions in the model.

(A color version of this figure is available in the online journal.)

between the theoretical 200 km and 2000 km (see also Figure 19(d)) spectra. The 200 km aperture spectrum of the theoretical model samples both the coldest (~20 K) part of the coma and a fairly optically thick part, with a P/R ratio $\gtrsim 1.8$ (some of which is due to low temperature, not only optical thickness). Thus, in conjunction with our low temperature, a factor of a few times greater density than that theoretical model (and corresponding increase in optical thickness) seemed a reason-

CO 1–0 Band; Q= 1×10^{27} s⁻¹ P/R Ratio vs. R (Phase angle=90°, Multiple Azimuthal angles)



Figure 22. For $Q_{CO} = 10^{27} \text{ s}^{-1}$. Ratio of *P*-branch vs. *R*-branch total brightness vs. *R* (impact parameter) for phase angle = 90° and for multiple azimuthal angles. Profiles of azimuthal angles show minimal variation for this case and overlap, appearing *nearly* indistinguishable, except inward of ~40–50 km. (Profiles are indicated by color coding in the online version.) "Sawtoothed" appearance of the plot is due to the division into discrete regions in the model. (A color version of this figure is available in the online journal.)





Figure 23. For $Q_{\rm CO} = 10^{28} \, {\rm s}^{-1}$. Ratio of *P*-branch vs. *R*-branch total brightness vs. *R* (impact parameter) for phase angle = 90° and for multiple azimuthal angles. Profiles of azimuthal angles show some variation in this case, but those for 0°, ±45°, and 90° overlap each other entirely in the calculated profiles and almost entirely in the observed. (Profiles are indicated by color coding in the online version.) "Sawtoothed" appearance of the plot is due to the division into discrete regions in the model.

(A color version of this figure is available in the online journal.)

able starting point to match the observations. This would be somewhat greater than the estimate based on observations and the use of the "optically thin" *g*-factor (see Table 3).

4.2. Garradd CO Model Parameters

Based on preliminary production rates derived from those observations (see Table 3), we modeled all three species for Garradd, at a distance of 2 AU. The production rates and other model parameters used are listed in Tables 4 and 5.

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 Table 3

 Brightness and Derived Values from Observations of Comet Garradd, for H2O, CO2, and CO

| | Values for | C/2009 P1 Garradd | | | | |
|---|--|--|--|--|--|--|
| Aperture Sizes (km ²) | | | | | | |
| Species | 4210×2105 | 12630×10525 | 21050×18945 | | | |
| | Band integrate | ed avg. surface brightness (erg cm ⁻² s ⁻¹ sr ⁻¹) | 3 | | | |
| H ₂ O CO ₂ | 6.2×10^{-3} 2.9 × 10^{-3} 2.4 × 10^{-3} | 2.9×10^{-3} 1.5×10^{-3} 8×10^{-4} | 1.6×10^{-3} 8×10^{-4} 5×10^{-4} | | | |
| | Integrated average | flux of bands (erg cm ^{-2} | s ⁻¹) | | | |
| H ₂ O CO ₂ CO | $\begin{array}{c} 1.2 \times 10^{-12} \\ 5.8 \times 10^{-13} \\ 4.8 \times 10^{-13} \end{array}$ | $\begin{array}{c} 5.8 \times 10^{-13} \\ 3 \times 10^{-13} \\ 1.6 \times 10^{-13} \end{array}$ | $\begin{array}{c} 3.2 \times 10^{-13} \\ 1.6 \times 10^{-13} \\ 1 \times 10^{-13} \end{array}$ | | | |
| | Average col | umn densities (cm ⁻²) | | | | |
| H ₂ O CO ₂ CO | $\begin{array}{c} 1.4 \times 10^{15} \\ 1.1 \times 10^{14} \\ 1.2 \times 10^{15} \end{array}$ | $\begin{array}{l} 6.4\times10^{14}\\ 5.8\times10^{13}\\ 3.9\times10^{14} \end{array}$ | $\begin{array}{c} 3.5\times 10^{14} \\ 3.1\times 10^{13} \\ 2.5\times 10^{14} \end{array}$ | | | |
| | Average p | roduction rates (s^{-1}) | | | | |
| H ₂ O CO ₂ CO | $\begin{array}{l} 2.4 \times 10^{28} \\ 1.9 \times 10^{27} \\ 2.0 \times 10^{28} \end{array}$ | $\begin{array}{l} 4.2 \times 10^{28} \\ 3.8 \times 10^{27} \\ 2.5 \times 10^{28} \end{array}$ | 3.9×10^{28} 3.5×10^{27} 2.8×10^{28} | | | |

Notes. Column densities and production rates are derived from observed brightness using the "optically thin" *g*-factor. From Feaga et al. (2014); see there for further details.

 Table 4

 Model Input Parameters for Modeling of Actual Observations of Comet Garradd for CO

| Model Parameters Used for C/2009 P1 Garradd | | | | |
|---|--|--|--|--|
| Mean nucleus radius | 3 km | | | |
| Heliocentric distance | 2 AU | | | |
| Heliocentric speed | 14.5 km s^{-1} | | | |
| T _{surface} | 40 K (tested 20-100 K) | | | |
| Expansion speed V_{exp} | 0.5 km s^{-1} | | | |
| $Q_{\rm CO}$ | $3.2 \times 10^{28} \text{ s}^{-1}$ | | | |
| $Q_{\rm H_2O}$ | $4.6 \times 10^{28} \text{ s}^{-1}$ | | | |
| Band center wavenumber | 2149 cm^{-1} | | | |
| Band center Einstein A | 33 s^{-1} | | | |
| Highest rot. level, J_{max} | 20 | | | |
| Solar flux (at 2 AU) | $6.25 \times 10^{12} \text{ photons cm}^{-2} \text{ s}^{-1} \text{ cm}^{-1}$ | | | |
| $\sigma_{ m rot}$ | $3.2 \times 10^{-15} \text{ cm}^2$ | | | |

We used a simple spherical model without including any coma morphology. We used a convolution and pixel binning simulating that of the *Deep Impact* HRI instrument, with $\lambda/\delta\lambda \sim 200-330$ (see Hampton et al. 2005).

4.3. Garradd CO Model Fitting

We tested a range of CO production rates beginning with the large-aperture optically thin value of $Q_{\rm CO} \sim 2.7 \times 10^{28} \, {\rm s}^{-1}$ and up to $4 \times 10^{28} \, {\rm s}^{-1}$. In conjunction with the best-fit temperature, $Q_{\rm CO} = 3.2 \times 10^{28}$ yielded the closest total brightness values to the data.

Fitting the temperature proved crucial to fitting the data with the model. Villanueva et al. (2012) measured a rotational temperature around 40 ± 7 K (1 σ) for Garradd at 2 AU for several species (within ~3000 km of the center of the comet, judging from the spatial profiles in their Figure 2; note, however,

 Table 5

 Brightness and Effective g-factor from Our Model of Comet Garradd, for H2O, CO2, and CO

| Mode | el ("best-fit") Values | for C/2009 P1 Garr | add | | |
|--|------------------------------------|--------------------------------|----------------------|--|--|
| Species | Production Rate (s ⁻¹) | | | | |
| H ₂ O | | 4.6×10^{28} | | | |
| CO_2 | 4.1×10^{27} | | | | |
| СО | 3.2×10^{28} | | | | |
| Aperture sizes (km ²) | | | | | |
| | 4210×2105 | 12630×10525 | 21050×18945 | | |
| Aperture avg. band total surface brightness | | | | | |
| | | $(erg cm^{-2} s^{-1} sr^{-1})$ | ¹) | | |
| H ₂ O | 7.9×10^{-3} | 2.6×10^{-3} | 1.6×10^{-3} | | |
| CO_2 | 4.2×10^{-3} | 1.4×10^{-3} | 8.3×10^{-3} | | |
| CO | 2.7×10^{-3} | 8.4×10^{-4} | 5.1×10^{-3} | | |
| Band total <i>g</i> -factor <i>at</i> $2 AU (s^{-1})$ | | | | | |
| H ₂ O | 5.2×10^{-5} | 6.6×10^{-5} | 6.9×10^{-5} | | |
| CO_2 | 4.9×10^{-4} | 6.2×10^{-4} | 6.5×10^{-4} | | |
| CO | 4.4×10^{-5} | 5.4×10^{-5} | 5.6×10^{-5} | | |
| Band total g-factor at $I AU(s^{-1})$ | | | | | |
| H ₂ O | 2.1×10^{-4} | 2.6×10^{-4} | 2.8×10^{-4} | | |
| CO_2 | 2.0×10^{-3} | 2.5×10^{-3} | 2.6×10^{-3} | | |
| CO | 1.8×10^{-4} | 2.1×10^{-4} | 2.2×10^{-4} | | |
| Percentage of optically thin <i>g</i> -factor (in parentheses) | | | | | |
| $H_2O(3.1 \times 10^{-4})$ | 68% | 84% | 90% | | |
| $CO_2 (2.8 \times 10^{-3})$ | 71% | 89% | 93% | | |
| $CO(2.4 \times 10^{-4})$ | 75% | 88% | 90% | | |

Notes. From Feaga et al. (2014); see there for further details. Note: "standard" *g*-factors are usually referred to with respect to comets' assumed heliocentric distance as 1 AU. We have presented both for the sake of clarity. (The 1 AU values are simply four times the 2 AU values.)

that their measurement was pre-perihelion and using other species). We tested temperatures within the range of the 40 ± 7 K measurements of Villanueva et al. (2012), and even some below the lower end of their 1σ range of 33 K. We found that these changes in temperature made some relatively small differences in the resulting spectra.

The best fit was achieved using a constant temperature of 40 K throughout the coma, in place of our initial profile (Figure 1). This is a gross but not unreasonable approximation. It is in rough agreement with Villanueva et al. (2012). Furthermore, our initial temperature profile has a fairly broad trough around its minimum of ~ 20 K that extends out to several hundred kilometers from the nucleus. It is reasonable that the warming of the coma after the minimum should be considerably slower/farther out in the coma at 2 AU than at 1 AU (since this warming is primarily due to photodissociation of H₂O) and probably stretches out the low-temperature zone discussed to a few thousand kilometers, or perhaps even farther. It should also be noted that the outer coma, where fluorescence dominates, is mostly unaffected by this approximation. Thus, our use of a constant temperature of 40 K makes the inner coma cold so as to fit the band profile in the inner coma, but has no effect on spectra of the outer coma where fluorescence dominates.

Due to noise considerations, the aperture-averaged band total brightness was deemed the most important measure of quality of model fitting, followed by peak values and band shape. See Table 3 for these brightness values and calculated column densities and production rates derived from them (see Feaga



Figure 24. 4210 km × 2105 km aperture-averaged spectra for $Q_{\rm CO} = 3.2 \times 10^{28} \, {\rm s}^{-1}$. Left side y-axis is aperture-averaged brightness in erg s⁻¹ cm⁻² sr⁻¹. Right y-axis is radiance in W m⁻² sr⁻¹ μ^{-1} . Vertical lines are individual line brightnesses. Continuous line is simulated HRI instrument spectrum. Totals are indicated on each graph.

Brightness, incl. D.Shift, CO 1-0 Bond; Carradd Q= 3.2×10^{3} s⁻¹; 10525x12630km Aperture, Phase= T_..._=33K $\lambda/\delta\lambda$ = 330



Figure 25. 12,630 km × 10,525 km aperture-averaged spectra for $Q_{\rm CO} = 3.2 \times 10^{28} \, {\rm s}^{-1}$. Left side *y*-axis is aperture-averaged brightness in erg s⁻¹ cm⁻² sr⁻¹. Right *y*-axis is radiance in W m⁻² sr⁻¹ μ^{-1} . Vertical lines are individual line brightnesses. Continuous line is simulated HRI instrument spectrum. Totals are indicated on each graph.

et al. 2014 for further details). Corresponding model results are shown in Table 5.

We present our model results in Figures 24, 25, and 26, as well as the model overplotted on the actual data in Figures 27, 28, and 29. Also see the values shown in Table 5 (and compare with observational data in Table 3).

Our "best-fit model" for CO used a production rate of $Q_{\rm CO} = 3.2 \times 10^{28} \text{ s}^{-1}$. This value is greater than the value that would be calculated (from the largest aperture) using the optically thin *g*-factor of $g_{\rm CO} = 2.4 \times 10^{-4} \text{ s}^{-1}$ (1 AU value), which would yield $Q_{\rm CO} \sim 2.7 \times 10^{28} \text{ s}^{-1}$ (for which a model was tried, but it produced a less close match to the data). Thus, some optical depth effects are still indicated for CO, even in the largest aperture size.

Figure 30 shows radial profiles for our "best-fit" model. The locations of the vertical lines indicating where the effective g-factor is 90% and 98% of the optically thin g-factor also

Brightness, incl. D.Shift, CO 1-O Band; Garradd Q= $3.2 \times 10^{29} \text{s}^{-1}$; 10000km Aperture, Phase=90 T = 47 K = 370



Figure 26. 20,000 km × 20,000 km (very close to 21,050 km × 18,945 km) aperture-averaged spectra for $Q_{\rm CO} = 3.2 \times 10^{28} \text{ s}^{-1}$. Left side y-axis is aperture-averaged brightness in erg s⁻¹ cm⁻² sr⁻¹. Right y-axis is radiance in W m⁻² sr⁻¹ μ^{-1} . Vertical lines are individual line brightnesses. Continuous line is simulated HRI instrument spectrum. Totals are indicated on each graph.



Figure 27. Model for all three molecules overplotted (red, in the online version) on Garradd small (2105 km \times 4210 km) aperture-averaged spectrum. From Feaga et al. (2014).

(A color version of this figure is available in the online journal.)

demonstrate that none of the spectra observed out to a radius of approximately 10,000 km are entirely free from optical depth effects. Furthermore, although these effects are relatively small at 10,000 km, they are considerably greater for the smaller aperture spectra.

4.3.1. Garradd Model Conclusions

The DI HRI Garradd spectra show optical depth effects, even for the largest aperture, which includes approximately a 10,000 km radius from the center of the comet. Our model results show that even a box aperture integrated out to that radius would underestimate the production rate by about 15% if an optically thin *g*-factor were assumed.

Numerically, these effects are also shown in Table 5, in the section showing percentage of optically thin *g*-factors; the values for the smallest aperture are about 50%-60% of the optically thin values. Thus, were one to naively use the optically thin *g*-factor to calculate production rates based on brightness values



Figure 28. Model for only CO overplotted (red, in the online version) on Garradd medium (10,525 km \times 12,630 km) aperture-averaged spectrum. See Feaga et al. (2014).



Figure 29. Model for all three molecules overplotted (red, in the online version) on Garradd large (18,945 km \times 21,050 km) aperture-averaged spectrum. From Feaga et al. (2014).

(A color version of this figure is available in the online journal.)

from the coma up to about 1000–2000 km radius, the resulting production rates would be incorrect by almost a factor of two!

In Figures 31, 32, and 33, we plot the residuals of the model and data, for the CO band. As can be readily seen, the level of noise on either side to the left or right of the band is of a similar magnitude to the residuals.

Our models have fit the data quite well in band total brightness, and fairly closely in peak values and band shape. The differences between the models and the data are at levels comparable to the noise and uncertainty of the observations themselves, particularly with respect to band shapes. The production rates used in these models are somewhat higher, but not dramatically so, than those that would be derived from the data based on the largest aperture assuming that the observations were optically thin. However, the production rate is significantly higher than what would be derived from the smallest aperture data assuming optical thinness.

Temperature also proved important in modeling band shape, to the noise-limited extent that shape fitting was possible. Our best-fit models use a fairly low temperature of 40 K throughout



Figure 30. Radial profiles for CO for Garradd. Upper frame: radial profile of band total brightness (in photons $s^{-1} cm^{-2} sr^{-1}$) vs. *R* (impact parameter, in km) for phase angle = 90° and for sunward and anti-sunward azimuthal angles. Column density is included on the left *y*-axis scale. Lower frame: effective *g*-factors. *g*_{eff}, brightness over column density, again plotted with angles corresponding to upper frame. The vertical lines represent the radial distance and column density at which *g*_{eff} is 90% and 98% of the optically thin value (along the anti-sunward direction, which has the lower *g*-factors). "Jaggedness" of the plots is due to the division into discrete regions in the model.

the inner coma, which at first may seem quite low at 2 AU, but it is in agreement with other observations (Villanueva et al. 2012.) This low temperature, in the collisionally dominated inner coma, works to fit the relatively narrow band shapes observed.

5. NEXT STEPS

We plan to present further useful results in forthcoming papers (A. M. Gersch & M. F. A'Hearn, in preparation) dealing with similar modeling to that presented here for H_2O and CO_2 , as well as a more in-depth treatment of CO alongside those species. We will present model results including morphology and comparison with the in situ spectral observations of the *Deep Impact* and *EPOXI* missions. The model and code have already been implemented to produce those results.

Further work will include several planned improvements to our model. A more accurate treatment of radial velocities and Doppler shifts in lines due to them is a highly desirable improvement. However, in as much as we are primarily looking at the overall *band* shape as opposed to individual line shapes, the effect of Doppler shifts on the spectra is expected to be less than if one were modeling specific lines (as is often the case for other spectral regimes). The effect of this neglect would be to increase the optical thickness, and therefore our results may be overestimating optical depth effects. If so, the effects we



Figure 31. Best-fit model's residuals for CO band plotted (red) on Garradd small (2105 km \times 4210 km) aperture-averaged spectrum (from Feaga et al. 2014). Within the band, the data and model are shown with dashed lines (black and blue, respectively, in the online version) to make viewing the residuals themselves clearer.



Figure 32. Best-fit model's residuals for CO band plotted (red) on Garradd medium (12,630 km \times 10,525 km) aperture-averaged spectrum (from Feaga et al. 2014). Within the band, the data and model are shown with dashed lines (black and blue, respectively, in the online version) to make viewing the residuals themselves clearer.

(A color version of this figure is available in the online journal.)

describe would still be observable, but for higher production rates than those modeled.

In addition to more accurate radial velocities, more flexible radial temperature and density profiles are planned, so as to be able to model deviations from a very simple Haser model (e.g., volatiles produced from icy grains or large chunks and not solely from the nucleus's surface, as per A'Hearn et al. 2011, and/or photodissociation of molecules, and corresponding creation of daughter species).

Computational limits are currently a limiting factor in how optically thick and how refined (in terms of granularity of conditions, in that more variation requires more regions) the modeled cases can be. As of now, the maximum production rates we can deal with are on the order of $Q \sim 10^{28} \text{ s}^{-1}$. We are planning to address these concerns with algorithmic



Figure 33. Best-fit model's residuals for CO band plotted (red) on Garradd large (20,000 km \times 20,000 km) aperture-averaged spectrum (from Feaga et al. 2014). Within the band, the data and model are shown with dashed lines (black and blue, respectively, in the online version) to make viewing the residuals themselves clearer.

(A color version of this figure is available in the online journal.)

improvements. Running the code on faster and more powerful computers is also a possibility.

6. CONCLUSIONS

We have demonstrated our model's usefulness in understanding emission spectra of cometary comae. There are several possible effects of optical depth that could lead observers to mistaken conclusions regarding the calculated abundances, or other characteristics, of species of interest. The moral of the story: ignore radiative transfer and optical depth effects at your own peril!

Although designed specifically with comets in mind, our model and code are versatile enough to be used in other radiative transfer problems as well. Parameters that define a specific comet model or other problem, including molecule of interest, size of nucleus and radial shells, production rate, morphology (if any), incident radiation, etc., are all fairly flexible. Thus, our adaptation of Coupled Escape Probability to an asymmetric spherical situation has created a very useful tool for modeling cometary spectra, as well as other spherical astrophysical phenomena.

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APPENDIX

ALGORITHM IMPLEMENTATION AND TECHNICAL DETAILS

We have coded the algorithm described above in the C++ language, using numerous functions from Press et al. (1992), primarily to implement numerical integration of functions (with odeint, stifbs, and associated functions) and solution of *N*-dimensional non-linear matrices with Newton's method (using newt and associated functions). The bulk of the coding, which implements the radiative transfer algorithm in spherical geometry, is our own.

A major practical limitation of our algorithm is the matrix size; since Newton's method requires (repeated) $O(N^3)$ matrix solving operations (for which newt uses the brute force approach of ludcmp and lubksb), the algorithm can get prohibitively slow for large matrices. For example, on an Intel Core computer (with CPU speed of 2.9 GHz and 7.6 GB of memory) running Scientific LINUX 6.3 (Carbon), when $N \gtrsim 15,000$, a solution may take one or more days. For greater sizes, it may take even a week. The matrix size equals the number of molecular levels used times the number of regions. The molecule (and band/s) being modeled determines the first value, with the latter value demanding to be increased with greater optical depths and production rates. Depending on the species of interest, the maximum practical production rates we can currently manage on such a system are of $O(10^{28})$ s⁻¹. The simplest workaround is to use a more powerful computer. Algorithms for solving sparse matrices faster than the above functions can also be used, and we have begun to explore this option.

In implementing the CEP method and our adaptation to spherical geometry, we have created C++ classes for diatomic and triatomic molecules. The object-oriented programming style of C++ lends itself ideally to being able to switch molecules easily. The Diatomic molecule class and its subclasses (currently implemented for CO and SiO) calculate energies and Einstein coefficients based on constants (taken primarily from Krupenie 1966, for CO) that are included in the code. The Triatomic class, which can actually be used for other polyatomic molecules as well (or the aforementioned diatomic molecules themselves, for that matter), must be provided with energies and coefficients from some outside source in formatted input files. We used the HITRAN database (see Rothman et al. 1998) to supply these values for CO_2 and H_2O . This approach has the versatility to handle many other molecules with a minimal effort of "data massaging" to get the data into the proper format. We have also created a large number of classes that encapsulate the spherical geometry and the attendant calculations. These are all "controlled" by the Comet class that reads parameters for a given case from a "comet definition file" (a text file of key/value pairs, essentially) and, using the above classes, sets up and runs the model for a given case.

Although designed specifically with comets in mind, our code is versatile enough to be used in other spherical radiative transfer problems as well. Straightforward input files describe all the required and optional parameters for a specific comet model or other problem, including molecule of interest, size of nucleus and radial shells, production rate, morphology (if any), incident radiation, etc.

The C++ code outputs a file containing a point-by-point line-by-line spectral mapping, as described above, for one or more specified viewing orientations. These data can then be presented in multiple formats as described above in Section 3. We have implemented this data presentation portion of the model using various short IDL programs that we have developed, each specifically for the purpose of producing a given type of graphical output.

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