THE DEVELOPMENT OF H 1 DISSOCIATION ZONES AROUND NEW H 11 REGIONS

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ABSTRACT

We present the results of computations for a model of the time development of H I photodissociation zones in the molecular gas around O and early B main-sequence stars and their associated H II regions. The computations are for a grid of values of stellar effective temperatures (T_{eff}) from 20 to 45 kK (spectral types B2.5 V-O5 V) and of ambient gas particle densities from 30 to 3000 atoms cm⁻³. We follow the conditions in the atomic gas in and behind the advancing dissociation front from an assumed stellar "switch-on" time until the ionization and associated shock front overtakes the zone of dissociation. A fraction of H₂ molecules which absorb photons in the Lyman-Werner bands are dissociated during the resulting electronic and vibrational excitation. The dissociation rates are much higher in regions close to the star where the UV energy density is sufficient to provide re-excitation before the molecules decay to the vibrational ground state. For most combinations of stellar type and gas density this ensures an initial rapid formation of an H I zone. The dissociation front then advances into the molecular gas on the time scale of the expansion of the H II region. As the H II region expands, the surrounding H I zone is eventually eroded by the advancing shock and ionization fronts.

The model calculations show the following features of atomic zones around H II regions: In low-density gas the unshocked H I zone will persist for up to half the main-sequence lifetime of the star, whereas in highdensity gas the zone will last only a few percent of the stellar lifetime. A star with a T_{eff} at the lower end of the range will dissociate to a radius several times the radius of the H II region, whereas the maximum width of the dissociation zone around a star at the early end of the range will be less than the ionized radius. The sizes and masses of both H II regions and their H I zones increase with decreasing density of the surrounding gas. For a given gas density, the total mass of atomic gas formed is not nearly as strong a function of stellar type as is the total mass of ionized gas. For a T_{eff} of 45 kK, the mass of H I at the time when the shock overtakes the dissociation front ranges from 25 M_{\odot} in gas of density 3000 cm⁻³ to 10⁵ M_{\odot} in gas of density 30 cm⁻³. The corresponding range for a T_{eff} of 20 kK is from 20 M_{\odot} to 2 × 10⁴ M_{\odot} . Although dissociation zones will form around all H II regions, they will be relatively more prominent where the exciting star has an effective temperature below 30,000 K. One can expect to detect photodissociated H I around young systems with exciting stars earlier than about spectral type B4.

Several heating and cooling processes are included in the model. The dominant heating processes are the dissociation itself in the advancing front, and the photoelectric effect on dust grains elsewhere. The most prominent cooling processes are infrared lines from H₂ molecules in molecular gas near the front, and the C⁺ line at 158 μ m in the dissociated atomic gas. Gas temperatures near young, rapidly advancing dissociation fronts may be as high as 1000 K, but values near 100 K are more typical of developed H I zones.

We discuss the detectability of H I zones. In about seven cases where sufficiently detailed observations are available, we compare the results of the model calculations with observations of 21 cm emission and absorption from H I zones surrounding H II regions. The exciting stars in these observations span the range from B5 to O6. The modeling calculations are generally in accord with the observations and permit a more comprehensive interpretation.

Subject headings: H II regions — ISM: general — ISM: molecules

1. INTRODUCTION

Emission at 21 cm wavelength from atomic hydrogen associated with young clusters containing O and B stars was detected in a number of early observations (Wade 1957; Davies & Tovmassian 1963; Raimond 1966). The first systematic search for H I specifically associated with discrete H II regions was undertaken by Riegel (1967). This study revealed definite detections in four cases of 27 regions searched, and possible detections in a further seven regions. The resolution of these early observations (~10') was insufficient to show any detailed structure in the H I emission, or to separate associated clouds from the background of extended emission. Nonetheless, it was apparent that the regions were extended and quite unlike the expected thin shocked shells of H 1 just ahead of the ionization fronts (Lasker 1966).

Much of this early work preceded the full realization that much of the gas near star-forming and H II regions is in the form of molecular clouds. More recent observations of higher resolution (Roger & Pedlar 1981; Read 1981a, b; Dewdney & Roger 1982; Roger & Irwin 1982; Joncas et al. 1985) have determined that the associated H I is often in broad intermediary zones between the ionized and molecular components, and is almost certainly due to specific dissociation of H_2 by the ultraviolet radiation from the exciting star(s). In some instances the H I shows expansion velocities in the range 2–7 km s⁻¹. In regions for which some estimate of temperature can be made (e.g., Roger & Irwin 1982) the values in the atomic gas are in the range 100–300 K.

It is our intention in this paper to present results of modeling computations which can be easily compared with these observations and which, with new predictions, can provide a direction for future measurements.

The dissociation of H₂ occurs through a two-step process proposed by Solomon (Field, Somerville, & Dressler 1966) and outlined by Stecher & Williams (1967) in which molecules are initially excited to the first electronic level and to a number of vibrational levels by the absorption of Lyman-Werner band photons in the range 91-112 nm. In the prompt return to the electronic ground state, approximately 11% of the molecules acquire sufficient vibrational energy to dissociate. The remaining molecules cascade through the vibrational-rotational levels toward the vibrational ground state. For low levels of UV energy density, typical of the general interstellar radiation field, several studies (e.g., Hollenbach, Werner, & Salpeter 1971; Jura 1974; Federman, Glassgold, & Kwan 1979) considered the advancement of plane-parallel dissociation fronts into molecular gas clouds from the outside and the conditions which result when an equilibrium is established between dissociation and re-formation. The fronts advance at rates determined by the imbalance between the rate of destruction of H_2 molecules and the rate of re-formation of molecules on dust grains. A state of equilibrium may eventually be reached and a transition zone of H I and H_2 established. London (1978) investigated the time-dependent effects, including heating, as a plane-parallel dissociation front advances into molecular gas. For the case of a newly formed O5 star in gas of density $n > 10^3$ cm⁻³ Hill & Hollenbach (1978) studied the infrared spectral lines produced as a dissociation wave expands into molecular surroundings. More recently, Tielens & Hollenbach (1985a) have modeled the chemistry and heat balance for the one-dimensional equilibrium situation of intense UV radiation fields impinging from the outside on dense (10^3) $cm^{-3} < n < 10^{6} cm^{-3}$) neutral clouds.

These treatments of dissociation fronts are not readily applicable to the general case of a new star forming within a molecular cloud, for several reasons. First, the levels of dissociating UV radiation just outside the initial ionization boundary can be many orders of magnitude greater than the general interstellar value. The photon flux is then sufficient to re-excite molecules before they relax to the ground vibrational state (multiple excitation) through absorptions in additional Lyman-Werner band transitions, thus increasing the chance of dissociation (Shull 1978; Harwit & Schmid-Burgk 1983). Second, the r^{-2} diminution of the radiation field in the neighborhood of a star plays an important role. Last, but not least, many of the H I zones observed may be produced by relatively young stars for which insufficient time has passed for the establishment of an equilibrium between the dissociation and reformation processes. Indeed, under some conditions full equilibrium may not occur during the lifetime of the exciting star, or it may be thwarted by factors such as density inhomogeneities or migration of the star relative to the surrounding gas. Even in the absence of such factors, the dissociation front may be overtaken by ionization and the associated shock before equilibrium is reached. Our model is specifically directed toward a description of the evolution of broad unshocked HI zones around newly formed stars and their H II regions.

In § 2 we will describe the input parameters and structure of

the time-dependent model, and the various processes included in the calculations. Results of the model computations are given in § 3 in the form of descriptive and observable parameters of the H I zones as functions of time for various stellar types and gas densities. In § 4 we discuss the implications of the model calculations and relate them to past and future observations.

2. THE MODEL

2.1. Assumptions

Our model represents a first-order attempt to follow the development of dissociation around a newly formed star and its H II region. We consider the approximation in which a star forms instantly within a molecular cloud of constant density, well shielded from the general interstellar ultraviolet radiation. We assume that the star maintains a constant luminosity throughout its main-sequence lifetime. Investigations of the later stages of protostellar collapse (e.g., Yorke & Krügel 1977) show that for nonrotating, nonmagnetic, spherically symmetrically collapsing protostars, the time spanned from the star first being able to significantly ionize ($U = 1.5 \text{ pc cm}^{-2}$, $N_L = 10^{44}$ photons s^{-1}) and dissociate to the stage when it reaches a main-sequence equilibrium is of order 10⁴ yr, and is not a strong function of the final stellar effective temperature. That is, more massive stars have further to evolve between these conditions, but the evolution proceeds more rapidly. If rotation and magnetic fields could be considered, it is likely that this time span would lengthen. The time for formation of an initial Strömgren sphere is approximately the reciprocal product of the recombination coefficient and the gas density, which varies from 5000 yr in gas of density 30 cm^{-3} to 50 yr in density of 3000 cm⁻³. Thus the "initial Strömgren sphere" will be in place when the main-sequence lifetime begins. For the purposes of the model, we assume that the Strömgren sphere and the main-sequence star are in place at t = 0.

The two main independent variables in the model are the effective temperature of the star (which corresponds to the main-sequence stellar type) and the density of the circumnebular gas in the parent molecular cloud. The values of many other less important parameters which can be varied in the model are listed together with their default values in Table 1. However, the results presented in § 3 make use of these values.

Our calculations assume spherical symmetry, and conditions in the surrounding medium are expressed as functions of both radius and time. We assume that all stellar radiation in the sub-Lyman continuum ($\lambda > 91.2$ nm) emerges from the H II region and is available for dissociation and heating. Lyman- α radiation emerging from the H II region is ignored.

2.2. Overall Structure of the Model

The structure of the modeling program is illustrated in the block diagram in Figure 1. For a given set of initial conditions, calculations are made at increments in radius from the ionization boundary outward within an outer loop incremented in time. The determination of the grid increments in radius and time is critical to the effective operation of the program. In the region of the advancing dissociation front, the intervals, in radius and time, must be sufficiently fine to portray accurately and follow changes in rates of dissociation, re-formation, ionization, recombination, heating, and cooling. Increments in time were determined empirically and were considered sufficiently fine when further subdivision resulted in no significant 538

TABLE 1										
DEFAULT VALUES OF MODEL PARAMETERS										

Parameter	Value
Total column density corresponding to 1 mag	
of visual extinction $(N_{1 \text{ mag}})$	$2.0 \times 10^{21} \mathrm{cm}^{-2}$
Re-formation rate of H ₂ molecules	
on dust grains (R)	$3.0 \times 10^{-17} \mathrm{cm}^{-3} \mathrm{s}^{-1}$
Photoelectric efficiency factor (y _{eff})	0.1
Dust-grain work function energy	8.0 eV
Grain albedo (a)	0.5
Grain scattering angle cosine	0.5
Cosmic-ray ionization rate (ζ_0)	$1.0 \times 10^{-16} \mathrm{s}^{-1}$
Carbon ionization rate $(\Upsilon_{c} \mu_{c})$	$3.28 \times 10^5 u_{10} \mathrm{s}^{-1}$
Sulfur ionization rate $(\Upsilon_{c} \mu_{c})$	$1.80 \times 10^6 \mu_{\rm ys} {\rm s}^{-1}$
Turbulent velocity width $(\delta V_{\rm b})$	$4.0 \mathrm{km s^{-1}}$
Abundances relative to hydrogen:	
Helium	0.1
Oxvgen	1.6×10^{-4}
Carbon	1.1×10^{-4}
Sulfur	1.0×10^{-5}
Silicon	1.5×10^{-6}
Iron	5.8×10^{-7}

change. Because the advancement of the dissociation front slowly decelerates, we have found that a time increment increasing exponentially with time is satisfactory. In radius, relatively coarse increments are acceptable in the largely molecular gas ahead of the dissociation front and in the predominantly atomic gas behind the front. In the region of the advancing dissociation front, however, a radius increment based on the slope of the density ratio, $n_{\rm H_2}/n_{\rm H\,I}$, in the previous time step is used. For each new time step the radius increments are recalculated so that the region of finest increments moves with the front. We note that there is a gross disparity between the very short length scales imposed by absorption in the Lyman-Werner lines and the longer scales for absorption of UV radiation by dust and r^{-2} diminution. This disparity can be six orders of magnitude in molecular gas.

For specific values of the initial conditions, including the main independent variables of gas density and stellar effective temperature, at each value of time and radius, the UV spectral energy densities corrected for radius (r^{-2}) , dust absorption and scattering, and line optical depths can be calculated for each Lyman-Werner band. The populations of the various vibrationally excited states of H₂ are determined entirely by these local UV energy densities. Rates of destruction for the molecules in the various vibrational levels and the general reformation of molecules on dust grains can then be calculated and applied to revise the densities.

Temperature-dependent processes, in particular several heating and cooling processes and three electron production processes, are contained in an iterative loop in a section of the program which treats the temperature in one of two ways: (1) If the total heating and cooling rates are almost equal after one time increment, the temperature is the equilibrium temperature, or (2) if the two rates are substantially different, the time increment is subdivided into steps such that the temperature can change by no more than 10% per step. New heating rates, cooling rates, and ionization balance are calculated for each substep in the inner loop, and the procedure is continued until the next main time increment.

Ionization balance (i.e., the densities of C^+ , S^+ , H^+ , and electrons) is determined iteratively to give a consistent solution for electron density in each of the three ionization/

recombination equations (see § 2.8). It is considered that a solution has been reached when the electron densities given by the production equations are consistent to within 0.1%.

All calculated parameters for the specific radius and time, including accumulated column densities, are stored and retrieved where necessary for calculations at subsequent points. For each time step, calculations continue to a radius where the density ratio $n_{\rm H\,I}/n_t$ reaches a limit, taken as 0.03%. For a given set of input parameters, calculations proceed until the advancing ionization/shock front effectively overtakes the more rapidly decelerating dissociation front.

2.3. Initial Conditions

We assume that the abundances of elements in the interstellar gas are as listed in Table 1. These values, from de Jong (1977), are somewhat depleted compared with solar abundances. We further assume that, prior to the formation of the



FIG. 1.-Block diagram of the structure of the modeling program

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exciting star, the circumstellar gas is well shielded from the general interstellar ultraviolet radiation and that atoms of carbon and oxygen, with similar abundances, are primarily in CO molecules. We adopt a dust-to-gas ratio of 1% by mass. Temperatures of 10–15 K are initially maintained by energetic electrons from cosmic-ray ionizations balanced mainly by cooling due to the $J = 1 \rightarrow 0$ transition of CO (Goldsmith & Langer 1978).

As the star forms and ionizes the surrounding gas, other changes occur in the gas on time scales short compared with the dissociation of molecular hydrogen. CO is readily dissociated in diffuse gas through the absorption of photons in bands in the range 89-110 nm (van Dishoeck & Black 1988; Viala et al. 1988). For most of these bands the probability of dissociation from the upper electronic state is high. The total rate of dissociation is determined by those lines with the shortest lifetimes in these upper states, by the self-shielding of the column density of CO, and by shielding through overlapping lines of H_2 . For the purposes of the model, we assume that the CO is predissociated. Carbon atoms are kept ionized by continuum photons in the same energy range (E > 11.26 eV) as that required for dissociation of CO. The extent of this ionized carbon may be limited ultimately by dust absorption or a density boundary. Energetic electrons from the ionization of carbon will heat the molecular gas (de Jong 1977). A more important source of heat, however, derives from the photoelectric effect on dust grains (Watson 1972) in which energetic photons dislodge electrons from the grain surfaces, which escape with excess energy that is shared with the gas through collisions. Cooling in this H_2/C^+ region will be largely through fine-structure emission of C^+ at 158 μ m and rotational transitions of H₂.

2.4. Ultraviolet Radiation Spectrum and Diminution by Dust

The UV radiation densities for our model are derived from interpolations of the tabulated values of stellar flux calculated by Kurucz (1979) for model stellar atmospheres and from the values of main-sequence stellar radii given by Panagia (1973). Flux values for the range in wavelength from 91 to 316 nm, and in stellar effective temperature from 18,000 to 45,000 K, have been extracted from the tables. To limit the number of variables, only radiation densities for solar metal abundances and for log surface gravity equal to 4.0 ($T_{eff} \leq 35,000$ K) or 4.5 ($T_{eff} > 35,000$ K) have been used. A further discussion of the radiative output of this range of stars is given in § 4.1.

It is convenient to express the UV energy density, u_{λ} , in units of the mean interstellar radiation field. We use the value 4×10^{-16} ergs cm⁻³ nm⁻¹, estimated by Habing (1968) for $\lambda = 100$ nm as this unit value and refer to it as the "Habing field" or "Habing unit." Although the value was derived at a specific wavelength, we will express energy densities at all wavelengths in these units.

In the calculation of energy density at a given wavelength and distance from the star, the value is corrected for r^{-2} , and for dust extinction and scattering. Our estimates of the interstellar extinctions corresponding to given column densities of gas are taken from values interpolated from the table of average, normalized extinction $[A_{\lambda}/E(B-V)]$ as a function of wavelength listed by Savage & Mathis (1979), and converted to values of the extinction ratio, A_{λ}/A_v , with an assumed ratio of $A_v/E(B-V) = 3.1$. To convert from column density to magnitudes of extinction, we use the factor $N_{1 \text{ mag}} \equiv N_{\text{H}}/A_v =$ 2×10^{21} protons cm⁻² mag⁻¹. Corrections to the energy density for scattering by dust grains are made by using the concept of the "exclusion optical depth" described by Whitworth (1975). We have used his tables of the ratio τ_{exc}/τ_{ext} , where τ_{exc} is the exclusion optical depth and τ_{ext} is the optical depth due to extinction. The values that we have selected are appropriate to a radiative transfer model for the case corresponding to a grain albedo of 0.5 and a mean forward scattering angle cosine of 0.5.

This treatment of absorption and scattering is valid for plane-parallel geometry. A comparison with a more sophisticated code for spherical geometry in a typical case (C. Rogers 1991, personal communication) shows that we may underestimate the illumination by factors in the range 1.3–1.6, not a serious matter given the uncertainties of the absorption and scattering parameters.

2.5. Absorption by Hydrogen Molecules

Values of the energy density calculated as described above represent the UV intensity prior to any line absorption by molecular hydrogen. The optical depths in the lines are extremely high, thus preventing the use of unshielded absorption rates in calculations of dissociation rates. The method used here is based on the photon penetration probability and uses a combination of the treatments of de Jong, Dalgarno, & Boland (1980) and Shull (1978), which in turn are based on the methods of Avrett & Hummer (1965). The effective absorption rate of UV photons is the product of the penetration probability and the unshielded absorption rate.

The following expressions involving penetration probabilities and absorption rates are used in determining the populations of the vibrational levels and the rate of dissociation. A more thorough discussion of the expressions can be found in de Jong et al. The absorption cross section, $\sigma_{v \to v'}$, for a particular transition $v \to v'$ is $(\pi e^2/mc)f_{v \to v'}$ cm² Hz, where v and v' are the lower and upper states of the transition and f is the oscillator strength. The unshielded absorption rate, $B_{0v \to v'}$, is $(\lambda^3/hc)\sigma_{v \to v'} u_{\lambda v} s^{-1}$, where $u_{\lambda v}$ ergs cm⁻³ nm⁻¹ is the average UV energy density appropriate to a Lyman or Werner band, and σ is the cross section. The optical depth at the line center, $\tau_{v \to v'}$, in terms of the molecular column density out to this point, N_{H_2} , is $(\sigma_{v \to v'} N_{H_2})/(\pi^{1/2}\Delta v_D)$ where Δv_D , the Doppler frequency width of the Lyman-Werner line, is $(\delta V_D v)/c$. The quantity δV_D is the turbulent velocity width of the gas.

In the above relations, the values of $f_{v \to v'}$ have been modified to account on the average for rotational splitting of the Lyman-Werner lines. The expression given by Schadee (1967), modified with approximations for this application, yields a factor $(J_{\max} + 1)/(2J_{\max} + 1)$ which is applied to the values of $f_{v \to v'}$ given by Allison & Dalgarno (1970). J_{\max} is the highest rotational state which is assumed to be populated. We have assumed that only *R*-branch transitions occur. Since energy differences between adjacent rotational levels are only about 0.015 eV, the rotational levels can be populated by thermal collisions. We have assumed a value of 7 for J_{\max} , corresponding to an average gas temperature of about 1000 K, a value representative of that near the dissociation front. The overall effect of this rotational splitting is not large, reducing the $f_{v \to v'}$'s by a factor of about 0.5.

For $\tau_{v \to v'} < 2.5$, in the linear part of the curve of growth, the expression for the penetration probability, $\beta(\tau_{v \to v'})$, of a particular transition uses the first nine terms from a power-series expansion of Shull (1978):

$$\beta^{L}(\tau_{v \to v'}) = \sum_{n=0}^{\infty} \frac{(-1)^{n} \tau_{v \to v'}^{n}}{n!(n+1)^{1/2}}$$

In the square-root portion of the curve of growth, with $\tau_{v \to v'} \ge 2.5$, we use the form given by de Jong et al. (1980):

$$\beta^{\text{SR}}(\tau_{v \to v'}) = (1.84a + 1)^{-1} \\ \times \left\{ \frac{2^{1/2}}{e\tau_{v \to v'} [\log_e(\tau_{v \to v'})]^{1/2}} + \left(\frac{a}{\tau_{v \to v'}}\right)^{1/2} \right\}$$

where $a = 9.23 \times 10^{-3} (\pi^{1/2} \delta V_D)^{-1}$ is the Voigt parameter with δV_D in kilometers per second.

Figure 2 shows a plot of the penetration probability for these two regimes as a function of the optical depth at the line center. De Jong et al. (1980) include an additional term in the calculation of the penetration probability to allow for overlap of the wings of adjacent lines in situations where the optical depth at the line center, $\tau_{v \to v'}$, is greater than about 10⁵. We have found that this term is seldom required, for the following reason. In each increment of time in the model, calculation of the density of H I continues until the atomic density reaches a small fraction (0.0003) of the total density, at which point the τ 's have reached their highest values, which is almost always less than 10^5 . In a few specific cases optical depths as high as 10^5 were encountered in our model near the end of the evaluated time range at the outermost limits of the dissociation front. On these rare occasions the dissociation front had almost reached an equilibrium radius and had been overtaken by the ionization-shock front. The above expressions for penetration probability are strictly valid only for slab geometry. However, since most of the dissociation takes place in a shell of minute thickness compared with its radius, little error is expected to result.

In the modeling program the optical depths in the Lyman-Werner lines and their wings at a given radius are determined from the current column of H_2 in each vibrational state of the lower electronic level. The optical depths are converted to photon penetration probabilities through the curve of growth (cf. Fig. 2) for each Lyman or Werner line. For the determination of the new local populations of the vibrational states, the penetration probabilities for lines with a common lower level are averaged over all upper levels to yield values of $\beta^{av}(v)$.



FIG. 2.—Photon penetration probability as a function of the optical depth at the line center for the linear (*curve a*) and square-root (*curve b*) portions of the curve of growth.

These are used to further decrement the UV radiation densities for each lower level. In turn, these energy densities are used to interpolate the local H₂ vibrational population ratios from a table computed and stored in advance. We discuss the generation of this table in the next section. For calculations of the dissociation rate (§ 2.7), the penetration probabilities for each line, $\beta(\tau_{v \to v'})$, are used with no averaging other than that of the oscillator strengths over the J transitions.

2.6. Populations of the Vibrational States of H_2

Shull (1978) first drew attention to the fact that the rate of dissociation of molecular hydrogen will increase substantially if the bound vibrational states of the ground electronic level are populated. With values of the UV energy density that exist throughout most of the interstellar medium, virtually all excited molecules relax back to the ground vibrational state in times of order 10⁵–10⁶ s (Black & Dalgarno 1976), well before electronic re-excitation. However, in the regions just outside the ionization boundaries of young O and B stars, the UV intensity can be up to 10⁵ times more intense than the mean interstellar radiation field, and it is highly probable that an excited molecule will absorb another Lyman or Werner photon before completing the vibrational cascade. The decay from the higher electronic state is rapid, and this "multiple excitation" process effectively both repopulates the bound vibrational levels and, in 11% of the cases, results in decay to the vibrational continuum (i.e., dissociation).

We assume that the populations of the excited vibrational states at each radius element are unaffected by collisional deexcitation and are determined only by the UV energy density at that point. (The mean time between collisions is of the order of 1-5 yr for gas of density 300 protons cm⁻³, and is dependent on the square root of temperature and inversely on density). This approach permits populations to be determined by interpolation from a precalculated table of population ratios indexed to the energy density. The validity of this approach depends upon the populations reaching a steady state in a time which is relatively small compared with the "dissociation time," as reflected in the typical time increments used in the model.

The distribution of vibrational states in intense UV fields has been considered by Shull (1978). A quantitative determination of the populations of the states requires a set of differential equations in which all the entry and exit rates, listed in Table 2, are summed for each vibrational state in the ground electronic state. The following notation is used in Table 2: v denotes the vibrational state (in the electronic ground state $X^{1}\Sigma_{a}$) whose population is being evaluated; v'' denotes an arbitrary vibrational-rotational state in the electronic ground state; v' denotes an arbitrary vibrational-rotational state, in one of the upper electronic states, either $B^{1}\Sigma_{u}$ or $C^{1}\Pi_{u}$. V_{max} , the highest value of v or v'', is 14. V'_{max} , the highest value of v', is 36 for the Lyman transitions and 13 for the Werner transitions, except when the transitions are energetic enough to require photons with wavelengths shorter than the Lyman limit for ionization, 91.2 nm. The net fraction, Q(v), of the population of molecules which absorb Lyman-Werner photons and then end up in the v state is given by Shull (1978), in which the sum of the Q's are tabulated for the Lyman and Werner transitions, weighted by oscillator strength. Oscillator strengths, $f_{v'' \rightarrow v'}$, for the Lyman and Werner transitions, and the transition probabilities for subsequent decay, $A(v' \rightarrow v)$, have been taken from

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TABLE 2 Entry and Exit Terms for Determining Populations of Vibrationally Excited H_2^a

Transitions	Term
Entry	
Spontaneous transitions from a higher vibrational state	$\sum_{v''=v+1}^{V_{\max}} n_{v''} A(v'' \to v)$
Lyman transitions originating from v''^{b}	$\sum_{\substack{v''=0\\v_{max}}}^{V_{max}} n_{v'} Q_{L}(v'' \to v) \sum_{\substack{v'=0\\v'=0}}^{V_{max}} B_{0L}(v'' \to v')$
Werner transitions originating from v''^{b}	$\sum_{v''=0}^{\max} n_{v''} Q_{\mathbf{W}}(v'' \to v) \sum_{v'=0}^{\max} B_{\mathbf{OW}}(v'' \to v')$
Exit	
Spontaneous transitions to a lower vibrational state	$\sum_{v''=0}^{v-1} n_v A(v \to v'')$
Lyman absorptions	$n_v \sum_{\substack{v'=0\\v'=0}}^{v_{\max}} B_{\mathrm{OL}}(v \to v')$
Werner absorptions	$n_v \sum_{v'=0}^{r \max} B_{0\mathbf{W}}(v \to v')$
^a The notation is defined in the text	

^b Q is given by Shull 1978:

$$Q(v'' \to v) = \sum_{v'=0}^{V_{\text{max}}} f(v'' \to v') [A(v' \to v)/A_{\text{tot}}] / \sum_{v'=0}^{V_{\text{max}}} f(v'' \to v') .$$

Allison & Dalgarno (1970). Transition probabilities for vibrational transitions in the ground electronic state, $A(v \rightarrow v'')$, are from Turner, Kirby-Docken, & Dalgarno (1977). Also, because the solution is required only for an elemental volume, and the attenuation of the UV energy density, $u_{\lambda v}$, in the gas column from the star has already been applied, we have used the unshielded absorption rates, B_0 's, in the determination of local populations.

The set of equations $\partial n(v)/\partial t = (\text{entry rates}) - (\text{exit rates})$ can be solved by standard techniques. Since they are included separately in the model, the formation and dissociation rates (as entry and exit terms, respectively) have not been included in Table 2.

Figure 3 shows the steady state solution of the population equations for each of the vibrational levels v for UV intensities ranging from 1 to 10^5 Habing units. Note that about half of the molecules are in an excited state when the UV intensity is just over 10^3 Habing units. At a UV intensity of 10^5 Habing units, almost 90% of the molecules are in excited states. Since each different level of vibrational excitation opens up another band of Lyman-Werner lines, the "opportunities" for absorption of a Lyman-Werner photon (and for subsequent dissociation) increase approximately in proportion to the number of lines in a band. Strictly, this is true only in the limit when the populations of all vibrational levels are equal.

We have compared our fractional populations of molecules in various vibrational states with calculations of relative column densities of H_2 molecules in vibrational states calculated by Sternberg (1988) for a single energy density equivalent to 170 Habing units (his Table 1). The relative column densities in the excited states correspond closely to our values of fractional populations from Figure 3. Referenced to the total population, Sternberg's values are close to our predictions for 130 Habing units, a good agreement considering that the compared parameters are not identical.

Figure 4 shows the "stabilization time," derived from a timedependent solution of the population equations, plotted against UV energy density for the case in which all the H_2 is initially in the ground vibrational state. Similar curves will apply to other initial conditions. The criterion for stabilization used here is that the fraction of the population in the ground (v = 0) state has settled to within 1% of its final asymptotic value. Regardless of the initial conditions, the relative populations of the various bound states tends to stabilize in about 10^6 s.

The active region, in which these excited populations of H_2 exist, forms the advancing dissociation front. The time taken for the front to advance a distance equal to its own thickness



FIG. 3.—Fraction of H₂ molecules in each vibrational state for radiation densities ranging from the mean interstellar value to 10^5 times this value. 1 Habing unit = 4×10^{-16} ergs cm⁻³ nm⁻¹.



FIG. 4.—Time taken for the relative population in the ground state to stabilize to within 1% of its final asymptotic value (*curve a*) and to within 10% (*curve b*), for various values of the local UV energy density.

depends upon the detailed conditions beyond the ionization boundary but is almost always much greater than the corresponding stabilization time. This permits the use of the tabular data shown in Figure 3 for calculations of the dissociation rates.

2.7. Dissociation and Re-formation of H_2

We compute the photodestruction rate with an expression similar to the formulations of Shull (1978) and of de Jong et al. (1980). The rate D(v) appropriate to molecules excited from the various bound vibrational states in the ground electronic level is given by the relation

$$D(v) = \frac{\lambda^3}{hc} p u_{\lambda v} (2J_{\max} + 1) \sum_{v'=0}^{V_{\max}} \sigma_{v \to v'} \beta(\tau_{v \to v'}) s^{-1} ,$$

where p is the probability of an excited molecule decaying to the vibrational continuum (dissociating). The parameter $u_{\lambda v}$ is the local UV energy density in ergs cm⁻³ nm⁻¹, diminished by r^{-2} and general dust absorption and scattering, and averaged over the wavelength range appropriate to v. The term $(2J_{max} + 1)$ accounts for the number of rotationally split lines. The individual destruction rate for each level, D(v), is applied separately to the corresponding density of molecules in that level. D is not particularly sensitive to the temperature of the gas.

Stecher & Williams (1978) describe a second mechanism for photodestruction which will be operative if the UV energy density is sufficient to populate vibrational levels substantially above v = 4. The mechanism involves photoionization of the vibrationally excited molecules with continuum photons near 100 nm, followed by photodissociation of the H₂⁺ by radiation over a wide range of wavelength (Dunn 1968). Since we have not included this mechanism in our model, photodestruction rates for extreme UV energy densities will be underestimated.

Re-formation of molecular hydrogen is assumed to take place on dust grains (cf. Hill & Hollenbach 1978) at a rate proportional to the product of the density of atomic hydrogen, $n_{\rm H\,I}$, and to the density of grains, which in turn is proportional to the total gas density, n_i . The rate of formation, F, is given by

$$F = Rn_{\rm H\,I}n_t \,{\rm cm^{-3} \, s^{-1}}$$

in which the rate coefficient, $R = 3 \times 10^{-17}$ cm³ s⁻¹, includes a gas-to-dust mass ratio of 100.

As indicated in § 2.2, the size of radius increments used in the model is based upon the slope of the ratio $n_{\rm H_2}/n_{\rm H_1}$ in the previous time increment. The *initial* radius and time increments are determined as follows: The initial radius increment, Δr_i , is chosen to represent the length of a column of gas in which there is only a small fractional change, $\Delta D(v)$, in the dissociation rate along the column for a given transition. Using only the first two terms in the expansion of $\beta^{\rm L}$, an expression for Δr_i can be derived for a particular transition: $\Delta r_i = [2^{3/2} \Delta v_{\rm D} \Delta D(v)]/(\sigma_{v \to v'} f_{v \to v'} n_v)$. We have chosen the value of $\Delta D(v)$ to be 0.5. After evaluating Δr_i for each transition, the minimum value is used. For the initial time increment we have then chosen a value such that the density of H₂ in the first radius element is decreased by only 20%.

2.8. Ionization Balance

As sources of free electrons in the model, we have the two most abundant heavy elements, carbon and sulfur, which can be ionized in a radiation field longward of 91.2 nm, plus hydrogen, which is ionized by cosmic rays (de Jong 1977). As noted by de Jong, the number of electrons freed from dust grains is negligible. Ionization balance for an atomic species A is determined by a set of simultaneous equations of the form $(\Upsilon_A u_{\lambda A})n_{nA} = \alpha_A(T)n_{iA}n_e$, where $(\Upsilon_A u_{\lambda A})$ s⁻¹ is the photoionization rate in an UV energy density of $u_{\lambda A}$ ergs cm⁻³ s⁻¹ (averaged over the appropriate range of wavelengths); n_{nA} cm⁻³ is the density of the neutral species; $\alpha_A(T)$ cm³ s⁻¹ is the recombination coefficient at gas temperature T; n_{iA} cm⁻³ is the density of the ionized species; n_e cm⁻³ is the density of electrons. The Υ 's and α 's for the heavy elements and the α for H are from Black (1975) and are listed in Table 1. The UV energy is averaged over a wavelength range from 91 to 110 nm for carbon and from 91 to 119 nm for sulfur. The ionization rate for H is given by Spitzer & Scott (1969) in the form $\zeta_0[(1$ + χ_{He} (1 + Φ) + 2 χ_{He}], where ζ_0 is the primary ionization rate (adopted as 1.0 × 10⁻¹⁶ s⁻¹; see Table 1); χ_{He} is the abundance of He (adopted as 0.1); and Φ has been tabulated by Spitzer & Scott as a function of $n_{\rm H I}/n_e$.

2.9. Heating and Cooling Processes

Our model includes four heating mechanisms: heating from the photodissociation of H_2 itself, from the photoejection of electrons from dust grains, from the ionization of carbon atoms, and from cosmic-ray ionization. The photoejection of electrons from polycyclic aromatic hydrocarbon (PAH) molecules has been suggested as a significant source of heating in the interstellar medium (d'Hendecourt & Léger 1987). We have not included this heating in our models; to do so would require some knowledge of the abundance and composition of PAHs and of their ability to survive in regions of high UV intensity. Heating from the vibrational de-excitation of H_2 , following excitation by UV radiation, becomes significant only at densities near or above our maximum density (Sternberg & Dalgarno 1989) and has not been included.

Overall, the most important heating mechanism on both sides of the dissociation front is that resulting from the photoejection of electrons from dust grains (Watson 1972) discussed in some detail by de Jong (1977), Draine (1978), and de Jong et al. (1980). Electrons are ejected with energies in excess of that required to overcome a work function energy barrier, taken to be 8 eV (Table 1), plus that due to the net positive charge on

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the grain which has accumulated from previous electron losses. The grain potential must be determined before the heating rate can be evaluated. Following de Jong (1977), we numerically integrate the left-hand side of the following equation for photoejection/recombination, starting at the Lyman limit, $v_{\rm H}$, until it equals the right-hand side:

$$\frac{y_{\rm eff} c^2}{h} \int_{v_0}^{v_{\rm H}} \frac{u_{\lambda}}{v^3} \, dv = \left(\frac{2kT}{m_e}\right)^{1/2} \left(1 + \frac{V_g}{kT}\right) n_e \, ,$$

where y_{eff} is the photoelectric efficiency factor, taken as 0.1 (see Table 1); v_0 is the lower frequency limit for which photons are energetic enough to eject electrons; T is the gas temperature; m_e is the mass of the electron; V_g is the electrostatic grain potential; n_e is the electron density. The result yields v_0 , which can be used to evaluate the photoelectric heating rate:

$$\Gamma_{\rm pe} = y_{\rm eff} c^2 \int_{v_0}^{v_{\rm H}} (n_d \, \sigma_d)_v \, u_\lambda \left(\frac{v - v_0}{v^3}\right) dv \, {\rm ergs} \, {\rm cm}^{-3} \, {\rm s}^{-1} \, ,$$

where

$$(n_d \sigma_d)_v = \frac{(1-a)(A_v/A_V)}{1.086N_{1 \text{ mag}}} n_t \text{ cm}^{-1}$$

and $(n_d \sigma_d)_v$ is the effective cross-sectional area of dust particles per cubic centimeter as a function of frequency; n_t protons cm⁻³ is the gas density; a is the albedo of the dust; A_v/A_V is the ratio of extinction at frequency v to that in the V band (cf. § 2.4); $N_{1 \text{ mag}}$ is the column density for 1 mag of extinction in the V band (cf. § 2.4); the factor 1.086 converts from powers of e to magnitudes.

Heating due to the excess energy from dissociation of molecular hydrogen is taken to be 0.4 eV per dissociation event (London 1978). The heating rate is given by $\Gamma_{H_2 \rightarrow H} = 0.4 n_{diss} / \Delta t$ eV cm⁻³ s⁻¹, where n_{diss} is the density of H₂ dissociated during the last time increment and Δt is the length of the increment. This process is the major source of heat in the neighborhood of the advancing dissociation front.

Calculation of the heating from electrons resulting from the ionization of carbon also follows the method of de Jong (1977), but with specific estimates of the average UV energy density in the spectral range applicable to single carbon ionization (91–110 nm). The resulting heating rate is $\Gamma_{C\to C^+} = \Upsilon_C u_{\lambda C} n_C$ ergs cm⁻³ s⁻¹, where Υ_C is given in Table 1; $u_{\lambda C}$ is the UV energy density averaged over the appropriate range of wavelengths; n_C is the density of carbon atoms.

For cosmic-ray heating, present at a low level largely independent of the dissociation, we follow the method of de Jong (1977), with corrections for secondary electrons taken from Spitzer & Scott (1969) and for a cosmic-ray ionization rate of $1.0 \times 10^{16} \text{ s}^{-1}$ (Table 1).

Cooling of the gas occurs through excitation of C⁺, O, Fe⁺, Si⁺, and C through collisions with electrons, hydrogen atoms, and molecules. Energy is lost through line emission in the infrared at wavelengths ranging from 26 μ m (Fe⁺) to 610 μ m (C). We have used equations for cooling rates as outlined by Dalgarno & McCray (1972). For example, the cooling rate for C⁺ excited by H atoms is given by $\Lambda = 1.0 \times 10^{-24}$ $L_{\rm H}({\rm C}^+/T)n_{\rm H\,I}n_{\rm C^+}$ ergs cm⁻³ s⁻¹, where, in this case, the cooling efficiency, $L_{\rm H}({\rm C}^+/T)$ is tabulated as a function of gas temperature in Table 4 of Dalgarno & McCray. Their Table 4 contains similar tabulations for O and C. Cooling efficiencies for Si⁺ and Fe⁺ are given by equations (22) and (23) of Dalgarno & McCray. Equations for excitation of C⁺, O, Fe⁺, and

Si⁺ are given by equations (3), (10), (8), and (5), respectively. Collisional excitation of O, C, and C⁺ by H₂ molecules are included with rates assumed to be 25% of the corresponding rates for hydrogen atoms (Dalgarno & McCray 1972).

We also include rotational $(J = 2 \rightarrow 0)$ cooling of thermalized H₂ as given by equation (8) of Goldsmith & Langer (1978) and, for temperatures greater than 100 K, the various vibrational-rotational transitions of H₂ summarized in Table 1 of Hartquist, Oppenheimer, & Dalgarno (1980). Throughout the regions of interest we assume that CO is largely dissociated in the molecular gas. If this were not the case, there would be strong cooling due to collisional excitation of CO by H₂ molecules (Goldsmith & Langer 1978).

Temperature as a function of time is determined assuming ideal-gas behavior under constant-volume conditions: $\partial T/\partial t = \frac{2}{3}kn(\Gamma - \Lambda)$, where T is the gas temperature, t is time, k is Boltzmann's constant, n is particle density, Γ is the total heating rate, and Λ is the total cooling rate. As outlined in § 2.2, heating, cooling, and ionization balance are redetermined at each new temperature.

2.10. The Expanding H II Region and the Shocked Component of H I

Although our model is concerned primarily with the gas beyond the ionization and shock fronts of the expanding H II region, the evolving properties of the ionized and the gradually accumulating shocked atomic gas play a role in determining the conditions at greater radii. At each time increment we calculate the velocity of the advancing shock, V_s , with an expression derived from the pressure "jump condition" across the shock in a manner similar to that given by Spitzer (1978), but including a term for the thermal pressure in the H I region ahead of the shock:

$$V_{s} = \left[\left(\frac{k}{1 - \rho_{\rm II}/4\rho_{\rm I}} \right) \left(\frac{\rho_{\rm II} T_{\rm II}}{\rho_{\rm I} \mu_{\rm II}} - \frac{T_{\rm I}}{\mu_{\rm I}} \right) \right]^{1/2} \, \rm cm \, \, \rm s^{-1} \, ,$$

where k is Boltzmann's constant, and T, ρ , and μ are the temperature, density, and mean mass per particle in the atomic ionized regions. The velocity and time increment determine the radial increment. Assuming constant UV flux, the density in the H II region will decline with the -3/2 power of its radius (e.g., Spitzer 1978). Thus the radial column density and the total mass in the ionized gas can be calculated. Since the original density and radius and the new radius determine the total mass of gas within the shock radius, the mass of shocked gas and its column density can also be calculated. The changing column densities in the ionized, shocked and unshocked atomic regions inside the dissociation front are than available for the calculations of absorption.

Lasker (1966) has determined that the maximum thickness of the shocked H I layer should be about 10% of the nebular radius in the absence of radiative cooling and much thinner with effective cooling. We have not attempted to estimate the thickness of the layer but note that, because cooling through the 63 μ m line of [O I] and the 158 μ m line of [C II] is very efficient, the layer is expected to be thin.

We choose to terminate the model calculations at the time when the radius of the shock/ionization front reaches the radius of the dissociation front, essentially marking the end of the unshocked H I zone.

3. RESULTS OF THE MODEL COMPUTATIONS

Computations have been carried out for 30 discrete combinations of the two main independent variables, the effective temperature of main-sequence stars and the ambient gas density. Particle densities of 30, 100, 300, 1000, and 3000 protons cm⁻³ and effective temperatures of 20, 25, 30, 35, 40, and 45 kK constitute the discrete values. This range in temperature covers approximately the main-sequence spectral types from B2 to O5. Interstellar clouds with mean particle densities less than 30 protons cm⁻³ are unlikely to be sites of star formation, and, in any case, would probably be insufficiently shielded to remain undissociated by the general interstellar radiation field. Densities greater than 3000 protons cm⁻³, while common in the cores of clouds, will not be generally typical of mean values in molecular clouds on parsec-scale sizes.

3.1. Advancement of the Dissociation Front with Time

In Figure 5 we illustrate the radial profile of dissociated gas in advance of the ionization/shock front for the case of a star with an effective temperature of 30 kK embedded in gas of density 300 protons cm⁻³ for four discrete times separated by factors of approximately 10. The profile corresponding to the earliest time illustrates the very rapid formation of a substantial dissociated zone of thickness similar to the initial Strömgren radius. The second profile, corresponding to 7000 yr, shows the H I zone near the time when the ratio of the zone's outer radius to the radius of the H II region is close to a maximum. The third profile, for 6.5×10^4 yr, illustrates the zone near its maximum thickness (and radial column density) and shows the encroachment on its inner radius by the expanding H II region and layer of shocked H I. In the final profile, at 7.6×10^5 yr, the advancing ionization/shock front is close to overtaking the dissociation front.

Figure 6a shows, for circumnebular gas of density 300 cm^{-3} and embedded stars of various temperatures, the advancement with time of the point at which half the molecules are dissociated. For comparison, the radii of the expanding H II regions are also shown, and we follow the dissociation until the advancing ionization overtakes the dissociation front at what we term the "catch-up radius." The axes are logarithmic, and it can be noted that, although the ultimate radius of the dissociation front is not a strong function of stellar temperature, the proportionate thickness of the dissociation zone decreases sharply with increasing temperature. By contrast, Figure 6b shows the development of the dissociation zones surrounding a star of effective temperature 30 kK for various gas densities. It can be seen that the zone scales closely with the radius of the H II region, although the absolute thickness is much greater for lesser gas densities.

Figure 7*a* illustrates the catch-up radius for all the various combinations of density and effective temperature. It is apparent that this radius is principally a function of gas density. The corresponding times for the overtaking to occur are illustrated in Figure 7*b*, together with the corresponding lifetimes of the main-sequence hydrogen-burning phase for stars of various initial stellar temperatures inferred from the data of Maeder & Meynet (1989). Here we see that in low-density gas an unshocked dissociation zone will persist for a good fraction of the main-sequence lifetime, regardless of the stellar type, whereas for densities in excess of 200 cm⁻³ the zone may be shocked and ionized in less than 10% of the lifetime.



FIG. 5.—Profiles of the density of the unshocked H I vs. radius for four times in the evolution of an advancing dissociation front of a star of effective temperature 30 kK and surrounding gas of density 300 proton cm⁻³.

3.2. Maximum Radial Thickness of the Dissociation Zone

The maximum of the ratio of the outer radius of the dissociation zone (half-dissociation point) to the H II region radius as a function of effective stellar temperature and gas density is shown in Figure 8a. Values of this ratio vary from close to unity for hotter stars in high-density surroundings to values close to 10 for cooler stars in similar surroundings. For midtemperature stars this ratio is not a strong function of the surrounding gas density. The time at which this maximum ratio occurs is shown in Figure 8b to vary from very early times in high-density situations to values near 10⁵ yr in low-density gas. At all densities the maximum ratio occurs later for hotter stars. Figure 9a shows the maximum radial thickness of the H I zone for the various combinations of gas density and stellar temperature. For densities below 1000 cm⁻³ this maximum thickness is relatively independent of stellar temperature, varying from ~8 pc for densities near 30 cm⁻³ to ~0.5 pc for



FIG. 6.—Advancement with time of the radial point at which half the molecules are dissociated (*solid line*) and of the radius of the expanding H II region (*dashed line*), (*a*) for a gas density of 300 cm^{-3} with six values of effective temperature and (*b*) for a star of effective temperature 30 kK and five values of gas density.



FIG. 7.—(a) Radius at which the dissociation front is overtaken by the expanding H II region ("catch-up radius") and (b) time taken for the overtaking to occur, for various combinations of gas density and stellar effective temperature. The dashed line in (b) shows, for comparison, the main-sequence lifetime for the stars of various effective temperatures.

values near 1000 cm⁻³. The time at which the zone reaches maximum thickness declines with both increasing stellar temperature and increasing density as portrayed in Figure 9b. Since the combination of gas density and thickness determines the column density through the zone, we will defer further comment until this latter parameter is considered.

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3.3. Rates of Dissociation and Accumulated Total Mass

The initial rates of dissociation are generally two to three orders of magnitude greater than the net ionization rates at the advancing ionization front. Figure 10 shows how the rates decline with time for stars of various temperatures in gas of



FIG. 8.—(a) Maximum ratio of the radius of the dissociation front to that of the expanding H II region and (b) time at which a maximum occurs in the ratio, for various combinations of gas density and stellar effective temperature.





FIG. 9.—(a) Maximum radial thickness of the dissociated zone and (b) time taken to reach this maximum thickness, for various combinations of stellar effective temperature and surrounding gas density.

density 300 cm⁻³ and for stars of $T_{\rm eff} = 30$ kK (spectral type B0) in gas of various densities. The net ionization rates and the rates of increase in the net shocked components of H I accumulated as expansion proceeds are also shown for comparison. The initial dissociation rate is principally a function of stellar temperature, reflecting as it does the total number of dissociating photons, and is almost independent of the surrounding gas density. However, the initial rate does persist for a much longer time in the lower density gas, due in part to the lower rates of re-formation and the lower proportional change in the r^{-2} UV diminution. After ~ 10⁴ yr, significant amounts of H I are caught up in the shocked atomic shell, and eventually the rate at which gas is shocked exceeds that of new H I production.

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The cumulative effects of the dissociation rates are illustrated in Figure 11 with plots of total dissociated mass as functions of time for runs of stellar temperature and gas density. Also shown in these figures are the mass of the shocked component of the atomic gas and the mass of ionized gas within the H II region. The curves are carried to the point where virtually all the accumulated H I has been shocked. Although this point occurs much sooner for stars with higher effective temperatures, the accumulated mass at these points is primarily a function of the gas density, and varies only slowly with stellar temperature. The ratio of the mass of dissociated gas to the mass of ionized gas in the H II region at this point, however, is much greater for lower temperature stars and varies only slowly with gas density. These final or terminal masses of H I and the corresponding masses of H II are plotted for all calculated combinations of stellar temperature and density in Figure 12. A comparison of these plots shows clearly that the mass of ionized gas has a much greater dependence on the luminosity of the exciting star than does the atomic mass.

It is instructive to look at the mass of dissociated gas at an earlier point in the evolution of the H I zone for all combinations of density and effective temperature. Figure 13 shows

the total mass of H I and the mass of the shocked component at the point in each situation where the ratio of the H I zone radius to the H II region radius is maximum. It is clear that at these earlier evolutionary times (cf. Fig. 8b), the dependences of the amount of dissociated mass on both stellar type and ambient density are significant.

3.4. Radial Column Densities of Shocked and Unshocked H I

The radial column density in an evolving zone around an exciting star combines, by definition, density and thickness parameters. Figure 14 illustrates the variation with time of the radial column densities of the ionized gas, the shocked H I, and the unshocked H I for runs of stellar temperature (n = 300cm⁻³) and gas density ($T_{\rm eff} = 30$ kK). The radial column density of the ionized gas declines with time as the effect of reduced density due to expansion outweighs the increased radius and the contribution of the newly ionized gas. The maximum radial column density of the unshocked component of the dissociated gas is not a strong function of either stellar type or gas density, peaking for the parameters used in our model within a factor of 2 of a value $\sim 2 \times 10^{21}$ cm⁻². This parameter is plotted in Figure 15a for the full range of densities and effective temperatures. Note the linear ordinate scale and the small range of values. The turnover for higher densities and higher effective stellar temperatures is caused by the more rapid encroachment of the shock front in these particular situations. Figure 15b shows the corresponding times for the occurrence of the maximum column density of the unshocked H 1 component.

3.5. Heating, Cooling, and Temperature in the Dissociation Zone

The variation of the most important heating and cooling rates with radius in the completely and partially dissociated gas is displayed in Figure 16 for a logarithmic sequence of four times in the case of a star of effective temperature 30 kK in gas



FIG. 10.—Rates of dissociation as a function of time (solid line), rate of new ionization (dotted line), and rate of increase of shocked atomic gas (dot-dash line), (a) for a gas density of 300 cm⁻³ with six values of effective temperature and (b) for a star of effective temperature 30 kK and five values of gas density.



FIG. 11.—Total dissociated mass of H I as a function of time (solid line), mass of ionized gas (dotted line), and mass of shocked H I (dot-dash line), (a) for a gas density of 300 cm^{-3} with six values of effective temperature and (b) for a star of effective temperature 30 kK and five values of gas density.



FIG. 12.—(a) Final total mass of H I (at catch-up time) and (b) corresponding mass of H II for various combinations of stellar effective temperature and surrounding gas density.

of density 300 cm⁻³. The resulting temperature profiles are shown in Figure 17 for each time, along with the corresponding radial density profile of the atomic gas (cf. Fig. 5).

At the earliest time shown the newly dissociated gas is heated to temperatures near 1000 K by the excess kinetic energy of the dissociation products, raising the cooling rate (due in about equal proportions to infrared lines of C^+ and O) to a level more than an order of magnitude greater than the heating rate. In the partially dissociated gas just ahead of the front, however, cooling by rotational lines of H_2 dominates, keeping the gas almost in thermal equilibrium. (The sharp vertical line in Fig. 16 is at the position of the dissociation front, denoting the falloff of heating or cooling which is associated with H_2 .) For a cooling rate of 1×10^{-22} ergs cm⁻³ s⁻¹ and a temperature rise of 1500 K, a rough calculation yields a time of about 10⁴ yr for equilibrium to occur. In the radial profile for 7000 yr the temperature peaks near 400 K at the dissociation front and the effects of the gas cooling behind the front are



FIG. 13.—(a) Total mass of H 1 and (b) mass of shocked H I, at the point in each calculation where the ratio of the H 1 zone radius to the H II region radius is a maximum, for various combinations of surrounding gas density and stellar effective temperature.



FIG. 19.—Temperature of the atomic gas just head of the advancing shock and ionization front as a function of time, (a) for a gas density of 300 cm⁻³ with six values of effective temperature and (b) for a star of effective temperature 30 kK and five values of gas density.



FIG. 15.—(a) Maximum radial column density of the unshocked H I and (b) corresponding times of occurrence of this maximum column density, for various combinations of model gas densities and stellar effective temperatures.

clearly seen. C⁺ cooling has begun to dominate over O cooling. Although O is slightly more abundant than C⁺, the temperature sensitivity of O cooling is greater than that of C⁺ in the 100–1000 K range. The suppression of the heating rate near the ionization front, and the concomitant rises in temperature and cooling rate, are due to the accumulation of grain charge, reducing the energy of photoelectrons ejected from dust particles. In the partially dissociated gas, heating and cooling processes associated with H₂ are less dominant.

At 6.5×10^4 yr essentially all the completely dissociated gas has reached an equilibrium temperature near 100 K. Except near the dissociation front, the gas is heated mainly by the photoelectric effect on dust. The dissociation heating approximately doubles the gas temperature at the front, which now moves more slowly, with the gas cooling to equilibrium in a relatively narrow radial distance. Cooling by rotational lines of H₂ is no longer important. The radial profile for 7.6×10^5 yr shows most of the gas at an equilibrium temperature near 40 K with only a slight perturbation at the dissociation front.

A more detailed illustration of the heating and cooling processes is given in Figure 18 for t = 1000 yr. In addition to photoelectric and dissociation heating, cosmic-ray heating and heating due to ionization of carbon are shown. Neither is an important heating component, but both contribute to the electron pool. Dissociation and re-formation of H₂ contribute some heating in the purely atomic zone. Here H is the principal exciter of C⁺ and O, with electrons playing a minor role in the excitation of C⁺. Other combinations of exciter/coolants are much less important. In the partially dissociated gas, electrons and H₂ molecules have some importance at radii greater than 2 pc in the excitation of C⁺. Neither, however, dominate the H₂ rotational cooling except at very large radii.

In Figure 19 we show the variation of gas temperature with time for a traveling point in the H I gas just ahead of the shock and ionization fronts for runs of stellar effective temperature

and gas density. For most cases, the gas temperature is initially in the range 1000–2000 K during the time when heat released by the dissociation process is dominant. After the dissociation front has moved significantly outward, the gas at this traveling point attains a temperature determined mainly by the balance between the heating due to the photoelectric effect on dust grains and the C⁺ cooling. The minimum apparent in most curves is due to the decreasing importance of dissociation heating with radius and to the suppression of the photoelectric heating caused by the accumulated charges on the dust grains. As the traveling point moves outward, the accumulated charge lessens, allowing increased heating until we reach the point where dust absorption and r^{-2} diminution of the ultraviolet reduce the effectiveness of the photoelectric effect.

In the region near the dissociation front where heating from dissociation is most intense, there is considerable time dependence to the heating and cooling. The minimum "thickness" and minimum time for which a new temperature can be ascribed are determined by the mean free path of particles and the mean time between collisions, respectively. The mean free path in atomic material of density 300 cm⁻³ is about 7×10^{-6} pc. The mean time between collisions is 43.6 $T^{-1/2}$, where T is the temperature in kelvins. For temperatures ranging from 100 to 1000 K, the mean time between collisions ranges from 4.4 to 1.4 yr. Also, the lifetimes of the vibro-rotational states of H_2 between which cooling transitions occur are of the order of 0.01-0.1 yr, and dissociation of the coolant is happening rapidly here. Therefore, in a narrow region around the dissociation front no thermalized steady state is reached, and we expect that temperatures are indeterminate.

Sternberg & Dalgarno (1989) present a detailed treatment of heating and cooling in dense ($n_{\rm H_2} = 10^3 - 10^7$ cm⁻³) photodissociation regions for the purpose of predicting the infrared response of the molecular hydrogen component. They conclude that for densities below 10^4 cm⁻³, gas temperatures in



FIG. 16.—Profiles of heating and cooling rates in the (unshocked) gas for selected times for the case of a star of $T_{eff} = 30$ kK in gas of density 300 protons cm⁻³, 7000 yr after the formation of the initial Strömgren sphere. The times chosen are the same as those for Fig. 5, where the locations of the ionization and dissociation for the time chosen are the same as those for Fig. 5. The time of the ionization and dissociation are the same as those for Fig. 5. The time of the ionization and dissociation are the same as those for Fig. 5. The time of the ionization are the same as the same as those for Fig. 5. The time of the ionization are the same as t fronts are illustrated (see also Fig. 17). Only the rates for the three most effective cooling processes are shown. (In this figure all contributions to the excitation of C⁺ and O are summed.) Also, only the rates for the most effective heating processes are shown.



FIG. 17.—Profiles of the temperature of the gas (solid lines) in the (unshocked) gas for the same case and times as in Fig. 16. The corresponding radial density profiles of the atomic component from Fig. 5 are shown as dashed lines.

the regions are close to 100 K, independent of UV energy density, and in general agreement with the results of our model.

4. DISCUSSION

4.1. General Considerations

The model calculations show clearly the dependence of the H I dissociation process on stellar type, surrounding gas density, and the age of the star. As with an H II region, the size and mass of the H I zone increase with decreasing density of the surrounding gas. Similarly, earlier type stars have more photons available for both ionization and dissociation.

However, compared with the companion H II region, the size and mass of the dissociation zone is relatively less dependant on the effective temperature (and the concomitant luminosity) of the exciting star (Fig. 12). Qualitatively, this may be



FIG. 18.—Profiles of heating and cooling rates in the (unshocked) gas for the same case as in Figs. 16 and 17, 7000 yr after the formation of the initial Strömgren sphere. The dissociation front is at a radius of approximately 1.4 pc at this time. Heating and cooling rates are shown individually for each of the heating and cooling processes considered in the model. In the plot of cooling rates, labels of the form $H-C^+$ are to be interpreted as excitation of C^+ by collisions with H.



FIG. 14.—Radial column densities of the ionized gas (dotted line), the dissociated but unshocked H 1 (solid line), and the shocked H 1 (dot-dash line) as functions of time, (a) for a gas density of 300 cm⁻³ with six values of effective temperature and (b) for a star of effective temperature 30 kK and five values of gas density.

explained as follows. First, the mean energy of photons from later type OB stars is shifted toward longer wavelengths in the UV, emphasizing photons capable of dissociating but not ionizing. Second, there is the r^{-2} enhancement of the intensity of stellar UV just outside the ionization front for cases of small H II regions around stars of lower effective temperatures. Finally, the dissociation zones around earlier type stars are more rapidly eroded by the advancing ionization fronts.

The relative number of photons available for ionization and dissociation can be assessed with reference to Table 3, which lists as a function of stellar effective temperature (col. [1]) the number of Lyman continuum photons (col. [2]) and the number of photons in each of the Lyman-Werner bands corresponding to the bound vibrational levels (cols. [3]-[17]). Note, however, that although virtually all Lyman continuum photons will ionize, only photons with energies corresponding to Lyman lines for significantly populated vibrational levels will result in dissociation. Thus, Table 3 is most useful for comparisons, within a given band, of the relative numbers of photons from stars of various temperatures. The relatively large factor (about 10⁵) in the ratio of ionizing photons over the range of $T_{\rm eff}$ is apparently due mainly to differences in the amount of continuum absorption in the stellar atmospheres shortward of the Lyman ionization limit ($\lambda = 91.2$ nm). Differences in the amount of helium absorption may also play a role. On the other hand, the radiative output in the stellar spectra just longward of the Lyman limit where the dissociation bands are located, changes by a factor of only 170 (for v = 0) over the range of $T_{\rm eff}$ considered. Hence dissociation remains an effective process for stars which produce little or no ionization.

The evolution of an H I zone is somewhat more complex than that of an H II region. The rapid initial rate of dissociation due to multiple excitation in the Lyman bands ensures that a substantial zone of atomic gas, like the initial Strömgren sphere, will form within the time scale required for the new star to attain main-sequence equilibrium. For most cases the ultraviolet intensity at the dissociation front is such that multiple excitation will persist for some time and permit the relatively rapid development of an H I zone. As the H II region begins to expand, the dissociation front continues to progress into the molecular gas. The lower luminosity stars (e.g., B2) will eventually dissociate to radii of more than 5 times their ionization boundaries, whereas for earlier types (e.g., O5) the dissociation does not extend beyond 1.5 times the ionization radii. The width of the dissociation zone will begin to decline when multiple excitation is no longer effective and advancement of the dissociation front falls below the expansion rate of the shock and ionization boundary. Ultimately the shock front will over-

take the dissociation region. The layer of shocked H I will have a thickness and density limited probably by magnetic pressure. With sufficient compression, the high densities in the layer will promote H₂ re-formation resulting in a pressure reduction, further compression and accelerated cooling through H₂ rotational transitions. As a fraction of the main-sequence (hydrogen-burning) lifetimes, the end of the unshocked dissociation zone will occur at a time determined mainly by the density of the surrounding gas. For gas densities in excess of 1000 atoms cm⁻³ this time may be only a few percent of the main-sequence lifetime, whereas for densities less than 30 atoms cm^{-3} the H I zone may persist for more than half the stellar lifetime. Since the lifetimes of the stars in the range we consider vary over an order of magnitude, there will be a similar variation in the actual lifetimes of the associated dissociation zones for any given mean density in the surrounding gas

Conditions in the unshocked H I zone do not appear to reach an equilibrium state in which the net dissociation and re-formation rates are equal before the zone is overtaken. The following simplified expression for dissociation-re-formation equilibrium, similar to one given by Hill & Hollenbach (1978), can be numerically integrated from the ionization boundary at r_0 to a point where dissociation is almost complete:

$$n_{\rm H_2} = \frac{Rn_t^2}{2Rn_t + I_0(r_0/r)^2\beta N_{\rm H_2}^{-1/2}e^{-KN_t}} \,\rm cm^{-3} \,,$$

where n_t and n_{H_2} are the proton density and the density of H₂, respectively, and the N's are the corresponding column densities. R is the molecule re-formation rate, $I_0 = 0.23B_0 \text{ s}^{-1}$ is the unshielded dissociation rate at radius r_0 , and K is the absorption coefficient of the dust. This relation employs the simplifying assumption that all Lyman-Werner absorptions are from the ground vibrational state. For the case of $n_t = 300$ protons cm⁻³ and a $T_{eff} = 30 \text{ kK}$ the expression yields a radius of the dissociation front of ~ 3.2 pc, and a column density of ~ 2.9 × 10²¹ cm⁻². These values are similar to the corresponding model results at the time of catch-up.

In constructing our model, most of the assumptions we have made have been conservative ones in the sense that they would tend to underestimate the rate and extent of the dissociation. This is particularly true for the treatment of the ultraviolet illumination which ignores Lyman- α and secondary Lyman-Werner band photons, for the treatment of the rotational line splitting, and for the neglect of dissociation of H₂⁺ formed from the ionization of vibrationally excited molecules (Stecher & Williams 1978).

TABLE 3

COMPARISON OF RADIA	TIVE OUTPUT FROM	EARLY-TYPE STARS IN	IONIZATION AND	DISSOCIATION BANDS
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$\frac{T_{\rm eff}^{\ a}}{(1)}$	N _{ion} ^b (2)	$N_{v=0}^{c}$ (3)	$N_{v=1}$ (4)	$N_{v=2}$ (5)	$N_{\nu=3}$ (6)	$N_{v=4}$ (7)	$N_{v=5}$ (8)	$N_{v=6}$ (9)	$N_{v=7}$ (10)	$N_{v=8}$ (11)	$N_{v=9}$ (12)	$N_{v=10}$ (13)	$N_{v=11}$ (14)	$N_{v=12}$ (15)	$N_{v=13}$ (16)	$N_{v=14}$ (17)
20	0.0024	1.2	1.9	1.9	1.7	2.9	2.9	3.1	3.2	3.4	3.3	3.5	3.6	3.6	3.3	3.6
25	0.089	6.8	10.2	9.9	8.2	13.5	13.0	13.5	13.5	14.3	13.4	13.8	13.9	13.9	12.8	13.9
30	1.4	20.6	29.3	27.6	21.4	35.0	33.1	33.6	33.6	35.8	33.5	33.9	34.0	34.1	31.5	34.3
35	14	39.9	54.4	49.7	36.7	60.1	56.6	57.1	57.4	61.7	57.7	58.4	58.7	59.1	54.5	59.6
40	68	102.5	137.7	125.0	89.1	146.5	137.1	137.0	136.6	145.9	136.0	136.4	136.6	136.8	126.5	137.3
45	270	205.1	272.2	245.2	172.5	284.1	265.6	264.9	264.1	282.0	262.7	263.2	263.5	263.8	244.4	264.5

^a Units are 10³ K.

^b Derived from Panagia 1973. Units are 10⁴⁷ photons s⁻¹.

^c Integrated over dissociation bands using stellar fluxes from Kurucz 1979 and stellar radii from Panagia 1973. Units are 10⁴⁷ photons s⁻¹.

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4.2. Detectability of H 1 Zones

The general problem of observing any H I feature in 21 cm emission is that of being able to discern the feature from the background of widely distributed low-density atomic hydrogen kept dissociated by the general interstellar UV radiation. With sufficient resolution H I zones formed by the specific dissociation of molecular hydrogen can usually be identified by their special morphology relative to the associated H II region or far-infrared source. Ease of detection will be determined by the masses and column densities of the H I at the particular time in the zone's evolution. Clearly low-density surroundings favor large total masses and the length of time for which a zone will survive. On the other hand, greater surrounding gas densities will yield higher column densities at the time of peak prominence of an H I zone, making it, for a period, easier to discern against the general background. The stellar luminosity will largely determine the prominence of the H I zone relative

to that of the associated H II region. Stars with higher effective temperatures will produce extensive ionized regions with relatively thin zones of H I, whereas stars with lower effective temperatures will ionize much smaller regions but still produce relatively substantial atomic zones.

The state of the atomic gas is indicative of the mainsequence age of the star and its H II region. The unshocked H I zone develops early in the star's lifetime and is transformed on the time scale of the expansion of the ionized region to a narrow shocked layer, which is slowly eroded by ionization. The shock decelerates and postshock gas ultimately becomes a subsonic flow of ionized and atomic gas. With any decline in luminosity in the later stages of a star's main-sequence lifetime, recombination of this ionized outflow may occur and again be detectable as an atomic zone.

4.3. Comparisons of Observations with the Models

Observations of a number of H I zones described in the literature have yielded parameters which can be compared with our model calculations. Parameters for a selected group of these are summarized in Table 4. The table lists the density (n), radius (R), and mass (M) for the H II and H I components, the emission measure (EM) of the ionized gas, and the column density (N_1) and expansion velocity (V_2) of the atomic components for the sources described in the following paragraphs.

At least three examples of easily detected H I zones surrounding small faint H II regions are known. The first is that surrounding the star LkH α 101 and near its associated reflection nebula NGC 1579 and an elongated dark cloud. Observations of 21 cm emission (Dewdney & Roger 1982) show ~85 M_{\odot} of H I in a cloud ~3.5 pc across surrounding an H II region, detected in thermal continuum radio emission (Dewdney & Roger 1986), of approximately one-tenth the

linear size and comprising ~0.1 M_{\odot} of ionized gas. Highresolution observations show a prominent circumstellar component in the ionized gas which corresponds to a region of mass outflow (Purton et al. 1982). Densities in the H II region are close to an order of magnitude higher than in the area of the H I zone. Taking this factor into account, we have compared the measured parameters with model calculations for various combinations of density, stellar temperature, and age, and find the observations consistent with a star of effective temperature near 25 kK, gas densities varying from 1000 cm⁻³ near the star to ~100 cm⁻³ in the H I, and an age of $\leq 10^4$ yr. Since expansion of the ionized gas has not yet occurred, a negligible amount of the dissociated gas should have accumulated in a shocked shell. None was detected.

The second example is the H I cloud of $\sim 1.4 M_{\odot}$ recently discovered to be associated with the far-infrared source IRAS 23545+6508 (Dewdney et al. 1991). Observations have revealed weak continuum emission at $\lambda = 6$ cm (S $\simeq 1$ mJy), which is consistent with an H II region of mass $6.6 \times 10^{-4} M_{\odot}$ surrounding an exciting star of spectral type near B3 ($T_{\rm eff} \simeq 18$ kK). As with LkH α 101, the observations indicate a higher density $(n \simeq 300 \text{ cm}^{-3})$ in the ionized gas than in the H I zone $(n_{\rm H\,I} \simeq 130 {\rm ~cm^{-3}})$. Again, the results are consistent with our models for an age of $\sim 10^4$ yr. Similar associations of H I clouds with far-infrared emission probably hold out the best hope for detecting specific dissociation regions for which the H II emission is obscured in the optical and too weak for easy detection in radio continuum emission. The dust coexistent with the atomic gas is heated mainly by photons in the same energy range as those responsible for dissociation, so it is to be expected that, to a first order, the dust emission at 60 and 100 μ m will show a distribution similar to that of the H I.

A third case of an H I zone surrounding a faint H II region is that reported by Rodríguez et al. (1990) surrounding the star SVS 3 associated with the reflection nebula NGC 1333 at a distance of ~350 pc. The flux density of the thermal emission indicates that the star is of spectral type B3.5 ZAMS ($T_{\rm eff} \simeq$ 16.6 kK), although its bolometric luminosity suggests B5–B6 ZAMS. The mass of H I is 0.017 M_{\odot} , a factor of ~1000 greater than the ionized mass. The mean densities of the H I and the H II implied by the observations are both ~5000 cm⁻³, significantly higher than the densities for the two previous examples. Although the stellar and density parameters are just out of the range of our models, the observations seem consistent with extrapolations from the model predictions for excitation by a star of $T_{\rm eff} = 16.6$ kK in gas of this density, provided that the region is at a very early stage of its evolution.

An excellent example of a developed H I zone surrounding a known H II region is that associated with IC 5146, excited by the B0 V star BD $+46^{\circ}3474$ (Roger & Irwin 1982). In this case

TABLE 4 Comparative Observational Examples

Object	T _{eff} (kK)	$M_{\rm II}$ (M_{\odot})	EM (cm ⁻⁶ pc)	R _{II} (pc)	$n_{\rm II}$ (cm ⁻³)	M_1 (M_2)	(cm^{-2})	$R_{\rm I}$ (pc)	$n_{\rm I}$ (cm ⁻³)	Age (vr)	V_{Iexp} (km s ⁻¹)
		<1.4 × 10 ⁻⁵	> 1.2 × 105	0.0025	> 5000	0.017	6 × 10 ²⁰	0.03		- 103	
23545 + 6508	18	$< 1.4 \times 10^{-4}$ 6.6 × 10 ⁻⁴	6200	0.0025	> 3000 340	1.4	0×10^{10} 0.9×10^{20}	0.03	133	~ 10 < 10 ⁴	0
LkHα 101	25	0.1	10 ⁵	0.15	1000	85	13×10^{20}	1.7	100	104	0
Sh 187	30	7.3	10800	0.8	150	60	12×10^{20}	1.7	240	1.5×10^{5}	
IC 5146	30	9.8	7900	1.1	110	450	6×10^{20}	3.0	200	105	2.3
NGC 281	40	2200	6200	10	20	> 3500	1.1×10^{20}	40	20	105	6.0
Sh 142	45	4000	15800	13	30	~ 3000	4×10^{20}	13		10 ⁵	

the H II region comprises 10 M_{\odot} within a radius of 1.1 pc and is surrounded by a atomic zone of $\sim 450 M_{\odot}$ within a radius of \sim 3.5 pc. Evidence that the system is more evolved than the two regions cited above is that the mean density in the ionized gas is about a factor of 2 less than the mean atomic density $(n_{\rm H\,I} \simeq 200 {\rm ~cm^{-3}})$, plausibly as a result of expansion. The observed parameters are consistent with our model predictions for a star of effective temperature 30 kK and an age near 10^5 yr . At this stage in the development the model predicts that $\sim 5\%$ of the dissociated HI should be within the shocked shell advancing at approximately 5 km s^{-1} . The distribution of the H I emission in angle and radial velocity was interpreted (Roger & Irwin 1982) as indicating a general outward expansion of all the atomic gas at ~ 2.3 km s⁻¹. In light of this prediction, however, a distribution with a mainly quiescent component plus a small shocked component should be tested against the observations.

A rather similar example is the H I zone associated with the H II region Sharpless 187 as described by Joncas, Durand, & Roger (1991). The region, probably excited by a B0 star, is partially optically obscured by the associated molecular cloud. There is evidence of "champagne-type" outflows from the relative velocities of the molecular, atomic, and ionized components.

Comparisons of highly evolved H II/H I systems with the models are generally more difficult because of the expansion of the nebulae into diffuse and possibly irregular surroundings. H I zones may be fragmentary and incomplete. NGC 281 is an extended emission nebula excited by the O6.5 V star HD 5005 and the O8 V star HD 5005C. Associated H I was first detected by Riegel (1967) and mapped in detail by Roger & Pedlar (1981). The ionized gas extends to radii of ~ 10 pc and the atomic gas to ~ 40 pc. Densities for both components are near 20 cm^{-3} ^b. The extent and total mass ($\sim 2200 M_{\odot}$) of the ionized gas and the presumed stellar excitation suggest an age near 10° yr. At this time the model would predict that a substantial fraction of the dissociated gas is entrained behind the shock front, which would be advancing at a velocity in the range 3-6 km s⁻¹. The observations show ~3500 M_{\odot} of H I in a broad band extending over half the perimeter of NGC 281 centered to the southeast of the source. From the distribution in angle and velocity Roger & Pedlar have concluded that this emitting region is expanding outward at ~ 6 km s⁻¹. It is likely, then, that the shock and ionization fronts in an evolved H II region such as this have become convoluted and that, in projection, the postshock atomic gas appears as a broad band of emission. Atomic gas farther from NGC 281, but still clearly associated with it, shows a distinctly narrower profile in velocity.

The H II region Sharpless 142, excited principally by the O6 V star DH Cep in the open cluster NGC 7380, also shows associated atomic hydrogen in a partial fragmented shell (Joncas et al. 1985). The total mass of ionized gas, 4000 M_{\odot}, and that of the associated atomic component, ~3000 M_{\odot}, are comparable to the estimated ~5600 M_{\odot} of molecular gas (Joncas, Kömpe, & de la Noë 1988), indicating that the ionization and dissociation processes are rapidly engulfing the available material. From the estimated age of the cluster, ~2 × 10⁶ yr, and the stellar excitation ($T_{\rm eff} \simeq 45$ kK), our models suggest that virtually all the dissociated gas should have been overtaken by the shock front. The H I gas distribution is complex, but there is some indication from spectral profiles that it may be shocked.

A few other regions which show dissociated gas, such as

those toward the complexes W3 (Read 1981a) and W58 (Read 1981b), show evidence of more than one source of excitation and of components at various stages of evolution. It is therefore much more difficult to compare the observations of H I emission from these regions with the model predictions. However, H I in absorption of the strong continuum emission from these compact H II regions has been detected and has revealed the shocked atomic gas. In studies of H I in absorption toward Orion A, van der Werf & Goss (1989) detect three distinct components of H I: first, the atomic envelope of the associated background molecular cloud; second, a swept-up layer of gas which shares the same velocity field as the ionized gas; and third, what is probably an intervening layer of photodissociated gas not yet overtaken by the shock front. Van der Werf & Goss estimate that the ratio of column density in the unshocked component to that in the shocked component is about 2:1. For their parameters of stellar effective temperature in the range 40-45 kK and an ambient density in the range $300-1000 \text{ cm}^{-3}$, our model would predict a column density ratio between 1.7 and 3.8 for the estimated age of the Orion complex, 5×10^5 yr.

4.4. Related Observations in Other Bands

Since the dissociation process results from the radiative excitation of hydrogen molecules, concomitant fluorescence in the infrared will occur in the dissociation fronts as the molecules relax through vibrational-rotational levels. Black & van Dishoeck (1987) have modeled the radiative excitation process and have shown that it can be distinguished from the more common thermal collisional excitation by a significant population of vibrational levels $v \ge 2$. Intensity ratios of lines near $\lambda = 2 \,\mu m$ which reflect this difference have been used by Gatley et al. (1987) and Sellgren (1986) to show the presence of UVpumped fluorescence in a number of regions principally classified as reflection nebulae and excited by stars in the spectral range B1-B3. Hayashi et al. (1985) have also detected a radiatively excited component to the fluorescence near the Orion Nebula. However, with the exception of Orion, none of the other detections coincide with objects for which dissociation zones in H I have been mapped. Clearly some of the young regions with advancing dissociation fronts, such as SVS 3, LkH α 101, and IRAS 23545+6508, are prime candidates for searches for fluorescence, although the densities may be lower than for regions in which detections have so far been made.

Broad-band emission in the range 500–900 nm, termed "extended red emission" (ERE), has been detected in a number of reflection nebulae (e.g., Witt & Boroson 1990), often coincident with regions of H_2 fluorescence. Duley (1985) suggested that the emission is due to luminescence excited by high UV flux levels incident upon hydrogenated amorphous carbon grains. Duley & Williams (1990) note that the conditions of high flux, high H-atom abundance, and elevated temperatures likely to be found in young dissociation fronts are probably ideal for rapid rehydrogenation of grains, and hence for the detection of ERE.

Carbon is singly ionized by photons of $\lambda < 113$ nm, in the same energy range as the Lyman band photons responsible for dissociation. Since, however, the ionization is achieved with continuum photons, the process can advance into the molecular gas ahead of the dissociation. The fine-structure line of C⁺ at 158 μ m constitutes the major coolant of the regions either side of the front. This line has been observed with airborne telescopes in a number of transition zones between H II regions

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and associated molecular clouds (e.g., Russell et al. 1981; Lane et al. 1990). Tielens & Hollenbach (1985b) have modeled the emission in this line and several others to match observations of the Orion Nebula. Current detections of C⁺ emission are for compact regions of higher density than those considered in our model calculations, although column densities are similar. As sensitivities improve and imaging without the limitations of restricted chopper throw become possible, the extended diffuse H I zones will become amenable to study. Similar considerations apply to observations of other spectral lines in the farinfrared, in particular the 63 μ m line of [O 1], which will be a major coolant in the regions of young dissociation fronts with elevated temperatures due to dissociation heating. Also in the far-infrared, measurement of the Brackett and Pfund series in the atomic zones, particularly for very young objects, may be fruitful. Kwan & Alonso-Costa (1988) have modeled the processes which involve absorption of the sub-Lyman continuum (91-113 nm) to produce enhanced emission in Bra and Bry. The region of $LkH\alpha$ 101 is one of several which display strong Brackett and Pfund lines (Simon & Cassar 1984) but the broad line widths suggest that the emission is from stellar outflow material rather than from the diffuse H 1.

An inspection of the far-infrared continuum emission at 60 and 100 μ m in images of the extended diffuse H I zones observed with the IRAS satellite reveals emission regions similar in size to the dissociation zones. This is consistent with our knowledge that the dust component of the gas surrounding an H II region is heated primarily by the sub-Lyman UV photons in a similar energy range to that of the Lyman-Werner bands. Furthermore, for a star optically obscured on all sides, we would expect the integrated far-infrared luminosity of the region to be close to the stellar luminosity of the exciting star. The integral estimated from IRAS flux densities for the H I/IR source IRAS 23545+6508 has been used (Dewdney et al. 1991) to imply a B3 star as the source of excitation, consistent with the excitation parameter derived for the faint H II region detected in 6 cm continuum emission. The IRAS data should be used for first-order analyses of the variation of dust conditions in different H I zones and as a function of radius from the exciting star(s) within each region.

4.5. Refinements to the Modeling

For the purposes of this description we have deliberately restricted the model to default values of a number of parameters which could be varied. With minimal effort the sensitivity of the model to variations in these parameters could be tested.

Since our prime interest is in determining the evolutionary development of the various components of the interstellar gas and dust in the neighborhood of O and early B stars, it is of some importance to be able to model the time variation of luminosity and temperature (UV continuum spectrum) of the stars before, during, and following their main-sequence lifetimes. Recent models of the evolution of massive stars (e.g., Maeder & Maynet 1989) are now sufficiently detailed that this could be attempted. Of particular interest is the onset of dissociation and ionization as a new star approaches the main sequence.

Our assumption of constant luminosity during the mainsequence lifetime needs scrutiny. A decline in luminosity or effective temperature, perhaps due to substantial mass loss, could result in a retreat of the ionization front, leaving a recombined H I zone with outwardly directed momentum. A similar situation may also arise at the end of the mainsequence lifetime, although we would expect it to be more difficult observationally to relate recombined gas concentrations to particular exciting stars at this stage.

We have assumed constant gas densities in the present description, although such an assumption is not realistic. The present model is capable of treating a specified monotonic density decline, and consideration should be given to extending the model to arbitrary density distributions. Certainly, some investigation of the role played by the portion of a protostellar cloud which has escaped collapse could be fruitful. Such circumstellar gas is likely to be of much higher density than the general surrounding medium and will be the first to be affected by the stellar radiation. The compact component of the H II region of LkH α 101 (Dewdney & Roger 1982) is probably the ionized remnant of such a cloud.

Our present treatment does not adequately consider the very late stages of the advancement of the shock and ionization front into the dissociated gas. Depending upon the degree of compression in the shocked H I shell, re-formation of H₂ molecules may possibly occur here before the so-called catch-up time and even alter the penetration of the ultraviolet to the unshocked gas beyond. With realistic estimates of magnetic fields, which are likely to limit the pressures and densities in the shocked shells, the model could be extended to include these effects. In this regard it is interesting to note that none of the observations of H I zones *in emission* appears to show a narrow zone, even in cases for which the detected expansion of the atomic gas would suggest that the H I has been shocked.

Star formation near the edges of molecular clouds is commonplace, and blister and champagne models (Zuckerman 1973; Tenorio-Tagle 1979) have been developed to aid in the interpretation of the observations of such regions. An extension of our model to adequately accommodate the variations in density inherent in blisters and champagne flows would be a major undertaking, requiring a full treatment of the dynamics of ionized and dissociated components. In the present work we justify ignoring the dynamics of the atomic gas on the grounds that the pressure which would cause the dissociation zone to expand is typically a factor of about 8 less than that in the ionized region. This will not be the case in early times near the dissociation front, where heat of dissociation raises the gas temperature above 1000 K, or in the layer of newly shocked gas prior to cooling. Density or pressure discontinuities conducive to champagne flows will seriously affect the dynamics of the ionized gas, and to a lesser extent the surrounding neutral material. The inclusion of a comprehensive treatment of the time-dependent photodissociation process in hydrodynamic codes such as that of Bodenheimer, Tenorio-Tagle, & Yorke (1979) would provide valuable insight into the evolution of atomic zones in nonhomogeneous regions.

Finally, extensions to the model which will enable the prediction of other observable parameters in the dissociation front, in the shocked and unshocked components of the atomic gas, and in the associated dust component are of considerable interest. In particular, the intensities of the fluorescence lines of H_2 , the cooling lines of [C II] and [O I] at 158 and 63 μ m, and predictions of the continuum emission from the UV-heated dust are particularly relevant to observations employing current and planned instruments for the far-infrared.

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- Allison, A. C., & Dalgarno, A. 1970, Atomic Data, 1, 289

- Allison, A. C., & Dalgarno, A. 1970, Atomic Data, 1, 289 Avrett, E. H., & Hummer, D. G. 1965, MNRAS, 130, 295 Black, J. H. 1975, Ph.D. thesis, Harvard Univ. Black, J. H., & Dalgarno, A. 1976, ApJ, 203, 132 Black, J. H., & van Dishoeck, E. F. 1987, ApJ, 322, 412 Bodenheimer, P., Tenorio-Tagle, G., & Yorke, H. W. 1979, ApJ, 233, 85 Dalgarno, A., & McCray, R. A. 1972, ARA&A, 10, 375 Dauges, D. & Tournessing, H. M. 1963, MNRAS, 127, 45

- 370, 243

- 3 /0, 243 d'Hendecourt, L. B., & Léger, A. 1987, A&A, 180, L9 Draine, B. T. 1978, ApJS, 36, 595 Duley, W. W. 1985, MNRAS, 215, 259 Duley, W. W., & Williams, D. A. 1990, MNRAS, 247, 647 Dunn, G. H. 1968, Phys. Rev., 172, 1 Federman, S. R., Glassgold, A. E., & Kwan, J. 1979, ApJ, 227, 466 Field, G. B. Somerville, W. B. & Dressler, K. 1966, APA & A. 4, 200
- Federman, S. R., Glassgold, A. E., & Kwan, J. 1979, ApJ, 227, 466
 Field, G. B., Somerville, W. B., & Dressler, K. 1966, ARA&A, 4, 207
 Gatley, I., Hasegawa, T., Suzuki, H., Garden, R., Grand, P., Lightfoot, J., Glencross, W., Okuda, H., & Nagata, T. 1987, ApJ, 318, L73
 Goldsmith, P. F., & Langer, W. D. 1978, ApJ, 222, 881
 Habing, H. J. 1968, Bull. Astron. Inst. Netherlands, 19, 421
 Hartquist, T. W., Oppenheimer, A., & Dalgarno, A. 1980, ApJ, 236, 182
 Harwit, M., & Schmid-Burgk, J. 1983, ApJ, 266, 602
 Hayashi, M., Hasegawa, T., Gatley, I., Garden, R., & Kaifu, M. 1985, MNRAS, 215, 31P

- Hayashi, M., Hasegawa, T., Gatley, I., Garden, R., & Kaifu, M. 1985, MNRAS, 215, 31P
 Hill, J. K., & Hollenbach, D. J. 1978, ApJ, 225, 390
 Hollenbach, D. J., Werner, M. W., & Salpeter, E. E. 1971, ApJ, 163, 165
 Joncas, G., Dewdney, P. E., Higgs, L. A., & Roy, J. R. 1985, ApJ, 298, 596
 Joncas, G., Durand, D., & Roger, R. S. 1991, ApJ, submitted
 Joncas, G., Kömpe, C., & de la Noë, J. 1988, ApJ, 332, 1030
 Jura, M. 1974, ApJ, 191, 375
 Kurucz, R. L. 1979, ApJS, 40, 1
 Kwan, J., & Alonso-Costa, J. L. 1988, ApJ, 330, 870
 Lane, A. P., Haas, M. R., Hollenbach, D. J., & Erickson, E. F. 1990, ApJ, 361, 132
 Iasker, B. M. 1966, ApJ, 143, 700
- Lasker, B. M. 1966, ApJ, 143, 700

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REFERENCES

- London, R. 1978, ApJ, 225, 405
- Bondon, R. 1976, ApJ, 225, 405
 Maeder, A., & Meynet, G. 1989, A&A, 210, 155
 Panagia, N. 1973, AJ, 78, 929
 Purton, C. R., Feldman, P. A., Marsh, K. A., Allen, D. A., & Wright, A. E. 1982, MNRAS, 198, 321
 Raimond, E. 1966, Bull. Astron. Inst. Netherlands, 18, 191
- Read, P. L. 1981a, MNRAS, 194, 863
- 1981b, MNRAS, 195, 371
- Riegel, K. W. 1967, ApJ, 148, 87
- Rodriguez, L. F., Lizano, S., Cantó, J., Escalante, V., & Mirabel, I. F. 1990, ApJ, 365, 261

- ApJ, 365, 261 Roger, R. S., & Irwin, J. A. 1982, ApJ, 256, 127 Roger, R. S., & Pedlar, A. 1981, A&A, 94, 238 Russell, R. D., Melnick, G., Smyers, S. D., Kurtz, N. T., Gosnell, T. R., Harwit, M., & Werner, M. W. 1981, ApJ, 250, L35 Savage, B. D., & Mathis, J. S. 1979, ARA&A, 17, 73 Schadee, A. 1967, J. Quant. Spectrosc. Rad. Transf., 7, 169 Sellgren, K. 1986, ApJ, 305, 399 Shull, J. M. 1978, ApJ, 219, 877 Simon, M., & Cassar, L. 1984, ApJ, 283, 179 Spitzer, L. 1978, Physical Processes in the Interstellar Medium (New York: Wiley)

- Wiley) Spitzer, L., & Scott, E. H. 1969, ApJ, 158, 161
- Stecher, T. P., & Williams, D. A. 1967, ApJ, 149, L29
- Interview (2011)
 Interview (2011)

- Telens, A. G. G. M., & Hollenbach, D. J. 1985a, ApJ, 291, 722 ------ 1985b, ApJ, 291, 747

- Zuckerman, B. 1973, ApJ, 183, 863