EVOLUTIONARY MODELS OF INTERSTELLAR CHEMISTRY

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ABSTRACT. The goal of evolutionary models of interstellar chemistry is to understand how interstellar clouds came to be the way they are, how they will change with time, and to place them in an evolutionary sequence with other celestial objects such as stars. To this end, we present an improved Mark II version of our earlier model of chemistry in dynamically evolving clouds. The Mark II model suggests that the conventional elemental C/O ratio less than one can explain the observed abundances of CI and the non-detection of O_2 in dense clouds. Coupled chemical-dynamical models seem to have the potential to generate many observable discriminators of the evolutionary tracks. This is exciting, because, in general, purely dynamical models do not yield enough verifiable discriminators of the predicted tracks.

1. INTRODUCTION

Considerable success has been achieved in understanding interstellar chemistry using either equilibrium or pseudo time-dependent chemical models which hold the background physical conditions of density, temperature and radiation field intensity constant [see, for example, reviews by J. Black (1) and E. Herbst (2)]. This success inspires us to make deeper inquiries. We would like to know why interstellar clouds like L183 and TMC-1 have strikingly different chemical composition even though they have strikingly similar physical properties. We would also like to know whether there is any common thread through widely diverse clouds, i.e., diffuse clouds, dark clouds, clouds with embedded infrared sources. To satisfy these curiosities, we need to understand how clouds attain a given physical and chemical structure starting with simplest initial conditions, and how they change thereafter. Equilibrium or even pseudo time-dependent models, which assume fixed density, temperature and radiation field intensity are not the proper tools for generating this understanding. We need evolutionary models which attempt to study the chemical-dynamical evolution of interstellar clouds with time in a coupled manner.

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2. GOALS AND OBJECTIVES

The ultimate goals of evolutionary models are to elucidate how clouds came to be the way they are, to predict how they will change with time, and to place them with related celestial bodies (e.g. stars) in an evolutionary sequence. These ambitious goals are best achieved by fusing together advances made in small steps whose objectives focus on well defined segments of the grand task. Thus, one objective of evolutionary models would be to investigate whether diffuse and dark clouds may be considered as different evolutionary phases of the same interstellar gas which is gravitationally contracting from an initial diffuse to a final dense state on the verge of star formation. This investigation might also show whether chemical differences between cold dark clouds with similar physical properties can be attributed to the possibility that clouds may attain similar physical properties following different dynamical tracks. If the answer is in the positive, then we may hope to identify chemical compositional signposts of dynamical evolution.

3. APPROACH

To construct an evolutionary model, with the limited objective set forth above, one would start with a given mass of interstellar gas confined (for simplicity) in a suitably large sphere, so that it represents an initial diffuse cloud cloud of (say) $A_v = 0.5$. Ideally, one would then follow the gravitational collapse of this cloud by simultaneously solving equations of heat budget, hydrodynamics, chemical balance, and radiation transport. A noteworthy attempt of this short is that of Gerola and Glassgold (3), although their model cloud with initial $A_v=2$ was somewhat far from being really diffuse. The ideal approach is very demanding of computer resource, even if the hydrodynamics is simplified by neglecting ordered magnetic field and rotation (which introduce deviation from spherical symmetry), and the chemistry is limited to only those species which significantly influence heat budget and dynamics. It is therefore no wonder that all previous attempts at evolutionary chemical models [e.g. Suzuki et al. (4) and Kiguchi et al. (5)] considered isothermal clouds under either free-fall or arbitrarily delayed free-fall. More recent evolutionary model of Leung and Herbst (private communications) are also of this nature. Due to the extreme simplification of dynamics these models are only marginally useful.

The approach adopted by Tarafdar, Prasad, Huntress, Villere, and Black [hereinafter referred to as TPHVB (6)] follows a middle course. Like Gerola and Glassgold (3), they also neglected the effects of magnetic field and rotation, and solved the equation of motion containing only gravitational and pressure gradient forces:

$$(1/\rho)\ \partial P/\partial r + Gm/r^2 + \partial^2 r/\partial t^2 = 0 \qquad (1)$$

together with the the continuity equation for spherical geometry, and the equation of state:

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$$1 - 4\pi r^2 \rho \partial r/\partial m = 0 \qquad (2)$$

and

$$P = RT/\mu \qquad (3)$$

In the above equations the reduced mass $\mu = 1/\{f(i)/m_i\}$ with f(i) as the fractional abundance of the species i, and the temperature T depends on the density ρ, visual extinction A_v, and the fractional abundances of the coolants such as C, C^+, and CO. Ideally the chemical balance equations governing the abundances of the coolants should be solved simultaneously with equations (1) thru (3). TPHVB did not adopt this ideal approach. Instead, following the reasoning given in their paper, they adopted the more practical way of determining T from the formula:

$$T = 163 / (2.5 + \ln n_H - \ln [1 + 500 \exp (-1.8 A_v)]) \qquad (4)$$

Note that this formula produces steeply rising temperatures at the edge of model clouds. Whether we adopt the more practical or the ideal way of calculating T, the bulk of the chemical evolution can be followed independently of the dynamical evolution, because the vast majority of the chemical species do not appreciably influence the dynamics. Thus, TPHVB studied the chemical evolution using the time history of the density structure from the dynamical calculations. This enabled them to consider a large number (i.e., 90) of species and also a very large number (i.e., 1000) of reactions. Choices of the species and reactions were based on the earlier equilibrium models of Prasad and Huntress (7). Never before evolutionary models had considered so detailed chemistry. A good treatment of radiative transfer of the UV radiation is important due to self-shielding effects in H_2 and ^{12}CO. As a starter, however, useful results have been obtained (6) by neglecting CO self-shielding and by using simplified expressions for H_2 photodissociation (8).

4. INITIAL RESULTS FROM EVOLUTIONARY CHEMICAL MODELS

Almost all evolutionary models, whether they consider purely dynamical evolution or the coupled chemical-dynamical evolution, have shown that very massive or very cold clouds will gravitationally evolve towards states of higher density culminating in star formation. Furthermore, during their evolution they develop core-envelop structure. The density is highest in the core and decreases with increasing radial distance with an inverse power law [see Woolfson (9), Larson (10), McNally (11), Bodenhiemer (12), Gerola and Glassgold (3)]. TPHVB model, however, has gone one step further by extending these results to low mass warm diffuse clouds. This was possible because the steep rise of temperature at the edges in their model produced an inward pressure gradient force strong enough to assist gravity significantly, so that even low mass warm diffuse clouds collapse without needing any triggers such as thermal-chemical instability or initial compression by shock waves.

Results from TPHVB's dynamical and chemical calculations suggest the possibility that diffuse and dense clouds may be related and form

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families in the sense that a given mass of interstellar gas will exhibit the entire range of the observed diffuse and dense cloud properties as it passes through the various evolutionary phases. One family of diffuse and dense clouds may differ from another by virtue of few simple initial conditions such as mass and density. It also appeared possible that the spread in the observed abundances of an atom or molecule at a given A_v or n_H may be due to differences in the evolutionary tracks caused by the differences in the initial conditions. TPHVB's model was the only evolutionary model to include condensation of molecules onto the grains, albiet in a very simplified manner. Their results suggest that condensation of gas phase species onto the grains may be much less of a problem in dynamically evolving models than in static models. This is a direct result of the fact that dynamically evolving clouds spend most of their lifetime as diffuse clouds and the lifetime of the dense core steeply decreases with increasing density. Evolutionary models of interstellar chemistry would, therefore, put lesser demands on the desorption mechanisms, if the dense cores of interstellar clouds do not last long after reaching the density of 10^6 cm^{-3} [Prasad (13)]. A possible way to fulfil this condition is to assume that star formation occurs soon after the core density of 10^6 cm^{-3} is reached. IRAS detection of infrared sources in a large fraction of previously known dense cloud cores (14) appears to lend some support to the required assumption.

Summing up, the above initial results suggest that evolutionary models may have the potential to accomplish objectives set for them. However, much remains to be done. For example, we do not as yet know how would these models perform in the case of complex molecules, and in the case of a significantly slower collapse. We have therefore performed some experiments with an improved Mark II version of our previous TPHVB model. These are described below.

5. MARK II EVOLUTIONARY MODEL OF INTERSTELLAR CHEMISTRY

Any model of interstellar chemistry, whether evolutionary or static equilibrium, must at least satisfy the following basic observational constrain on few of the simplest members of the H-C-O family:
(i) Large CI abundances found even deep inside dense clouds so that N(CI)/N(CO) is between 0.01 and 0.1 throughout dense clouds (15,16,17) (ii) Non-detection of O_2 in dense clouds (18,19), and (iii) The ratio $N(C_2H)/N(CO)$ is on the order of 0.0001 throughout dense clouds (20). Using static equilibrium models, Langer et al. (21) and Herbst and Leung (22) have tried to explain the CI observations (15,16,17) on the basis of the possibility that elemental C/O ratio may be larger than unity in at least the clouds having large CI abundance. Unfortunately, the observational foundation for this possibility is only marginal, considering the relevant data presented by Tarafdar, Prasad, and Huntress (23). In addition, if the C/O abundance ratio is adjusted to values greater than one to model the observed N(CI)/N(CO), then the predicted abundances of C_2H, C_3H and C_3H_2 are greater than their observed values by 2 to 4 orders of magnitudes. [For example, the observed $f(C_2H) \sim 10^{-8}$ is

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quite smaller than the predicted values of $(1-2)\times10^{-7}$ and 2.7×10^{-6} in the models of Langer et al. (21) and Herbst and Leung (22). The observed $f(C_3H)$ on the order of 5×10^{-10} (24) is about four orders of magnitude smaller than the predicted value of 2.7×10^{-6} from Herbst and Leung (22).] We, therefore, continue to use the conventional C/O ratio less than unity in the Mark II version of our evolutionary model. For a better representation of the C and CO chemistry, we also include the photodissociation of CO by the dilute uv radiation field deep inside dense clouds. As discussed by Prasad and Tarafdar (25), this dilute uv radiation is generated by the cosmic ray excitation of the Lyman and Werner bands of hydrogen. Direct retrieval of CI from CO by the photodissociation is expected to enhance the abundance of neutral atomic carbon and the synthesis of complex molecules (22,26). To reduce O_2 abundance to a non-detectable level, we have channeled O into H_2O faster than into O_2 by assuming that water is the most predominant product in H_3O^+ ion recombinations, and that the $O + OH \rightarrow O_2 + H$ reaction has an activation temperature of 83K. Observed limits on the H_2O abundance in diffuse clouds suggest that water is probably the predominant product in the H_3O^+ recombinations (27). Our first assumption is consistent with this, given the uncertainties in the astronomical data. Our second assumption is also consistent with Black and Smith's (28) analysis of experimental data on the O + OH reaction.

The assumed efficient channeling of O into water has a potential conflict with the fact that water has not been observed in dense clouds under normal conditions. We have, therefore, further assumed that water freezes onto grains on every collision, and remains stored on them thereafter. In sharp contrast, we neglected freezing onto grains for all other species. The observed near constancy of the molecular abundances with the hydrogen density (29) suggests the existence of some very efficient, but presently unknown and unquantifiable, desorption mechanisms. Rather than consider condensation and either neglect or treat desorption in an uncertain manner, we have at this time chosen to ignore both processes for all species except water. Water was considered an exception, because it has the highest freezing point. We hope that our results will justify these provisional assumptions. Finally, the Mark II model includes almost all observed complex molecules and related ions and neutrals. Thus, we now have 180 species which participate in 1626 reactions. These species are mostly the same as in Leung et al.'s (26) model. Chemical reactions involving the additional species are also mostly from Leung et al., excepting that the rate coefficients for the radiative association reactions and H_3^+ recombinations are from Herbst (30), and Smith and Adams (31) respectively. Depleted metal abundances were used to ensure low electron density.

6. RESULTS FROM THE MARK II MODEL

Two sets of experiments were done with the Mark II model. In the first set the time evolution of the physical structure of the cloud was determined by the solution of dynamical equations (1) thru (3). This results

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in a "fast" collapse, so that model clouds evolve from initial diffuse to a final dense state with core density of 10^4 cm^{-3} in just a few million years (6). A well-known problem with the assumption that all material within molecular clouds of our galaxy is collapsing at near free-fall rate is that it leads to star formation rate at least an order of magnitude larger than the currently accepted value [Zuckerman and Palmer (32), Smith et al. (33)]. In the second set of experiments, therefore, the time evolution was arbitrarily slowed by a factor of ten uniformly to model a "slow" collapse. Clouds with different masses and initial densities were considered in each set of experiments. For comparison, some equilibrium models were also constructed at densities of 10^3 and 10^4 cm^{-3} and temperatures of 10 and 50K.

Figure 1 shows the results for C, and CO abundances in a cloud of $100M_\odot$ when it attained the core density of $10^4 cm^{-3}$ after evolving for 3MY. With the modified C and CO chemistry, the predicted abundances of C, CO, and C_2H are in good agreement with observations (15,16,17, 20) for the case C/O < 1. The opposite case of C/O > 1 tends to over-predict CI and C_2H abundances, the latter in a rather unsatisfactory

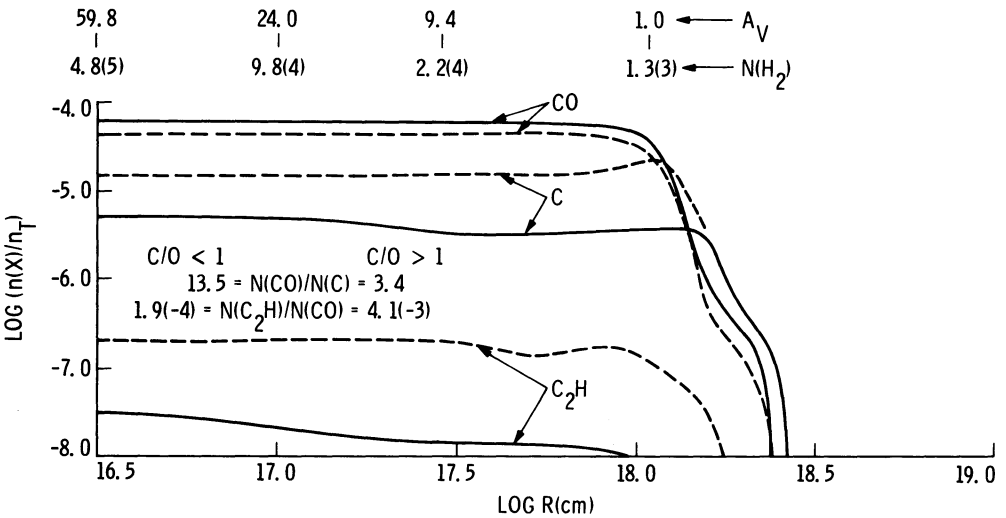

Figure 1. Variations of C, CO and C_2H abundances in a model cloud of $100M_\odot$ when it attained a core density of $10^4 cm^{-3}$ after evolving for 3MY. Solid and dashed lines are respectively for the two cases of C/O ratios less than and greater than unity. The radial variations of density and A_v at this epoch is represented by their values at selected radial distances given at the top of the figure.

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manner, considering the ratios of the column densities inserted in the figure. It is, therefore, concluded that the assumption of C/O > 1 is probably not necessary. Figure 2 shows our new results for O, O_2,and

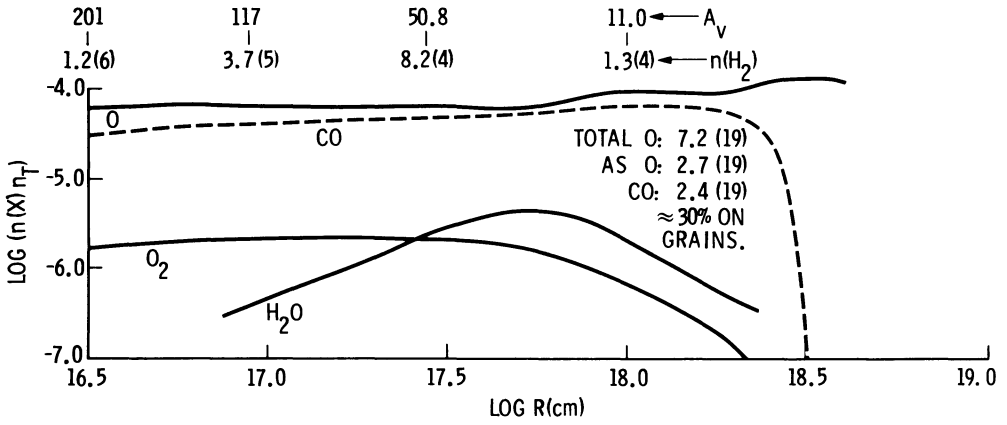

Figure 2. Variations of O, O_2, CO and H_2O in a model cloud of 1000 $M_\odot$ at 4MY for C/O < 1. Variaions of density and A_v are represented in the manner of Figure 1. The insert gives the column density of the various species.

H_2O in a model cloud of 1000$M_\odot$ at 4MY when the density at the center was 1.2×10^6 cm^{-3}. In agreement with its non-detection (18,19), the abundance of O_2 was every where low (< a few x 10^{-6}). The abundance of H_2O maximized at a density of a few x 10^4 cm^{-3}. Below this density H_2O abundance decreases due to rapid photodissociation. Above that density, the decrease in H_2O in the present case is due to its freezing onto the grains.

The effects of the slower rate of collapse can be seen from Table I. For the ten times slower collapse the fractional abundance of carbon and the N(CI)/N(CO) ratio decreased considerably relative to their values in the case of the fast, almost free-fall, collapse. Most of the decrease was found to have occurred in the densest core, which is in agreement with the observation that CI appears to avoid the dense core (17). Given this and the observed $f(C_3H) \sim 5 \times 10^{-10}$ and $f(C_3H_2) \sim (5\text{-}10) \times 10^{-9}$, (24, 34) it appears that the fast collapse of our previous model is probably farther from reality than relatively slower collapses. This is also suggested by many other molecules which can not be discussed here due to paucity of space. The new key point is that we have reached this conclusion on the basis of chemical considerations. Physical properties,

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Table I. Comparison of the Predicted Chemical Abundances in the Case of Slow and Fast Collapses. Note that a(b) = a x 10^b.

SPECIES	ABUNDANCE		SPECIES	ABUNDANCES	
	FAST	SLOW		FAST	SLOW
C	2(-5)	3(-6)	C_3H_2	3(-9)	1(-8)
CO	1(-4)	1(-4)	O	1(-4)	9(-6)
C_2H	5(-8)	3(-7)	O_2	4(-6)	3(-6)
C_3H	9(-11)	2(-10)	% of O on grains	30%	60%

such as the predicted velocity field, are not sensitive discriminator of the dynamical collapse. It is, therefore, exciting that the chemistry might possibly serve as signposts of collapse. Another example of the usefulness of chemistry is provided by a comparison of the observed and the predicted abundances of three complex molecules shown in Table II. The observed abundances are from TMC-1, which is currently thought to be a prototype of dark clouds without embedded infrared sources, and the theoretical abundances are from a variety of modeling experiments.

Table II. Comparison of Theoretically Predicted and Observed Abundances of a Few Complex Molecules. Note that a(b)= ax10^b.

SPECIES	OBSERVED ABUNDANCES FROM TMC-1	THEORETICAL PREDICTIONS FROM MODELS: EVOLUTIONARY		EQUILIBRIUM	
		$1000M_\odot$ (SLOW FAST)	$100M_\odot$ C < O C > O	$N=10(6)cm^{-3}$ A_v= 50 10K	50K
CH_3OH (Methanol)	1(-9)	3(-11) 4(-10)	9(-11) 6(-11)	2(-9)	2(-7)
CH_3CN (Methyl-cyanide)	1(-9)	5(-11) 5(-11)	3(-11) 4(-11)	4(-11)	3(-8)
CH_3COH (Acetyl-dehyde)	6(-10)	1(-7) 2(-8)	1(-7) 4(-8)	4(-7)	4(-9)

While the formation of CH_3OH and CH_3CN is initiated by the radiative association of CH_3^+ with H_2O and HCN respectively, CH_3COH is derived from the radiative association of CH_3^+ with CO. The large difference between the observed and the pedicted abundances of these neutral molecules in the evolutionary model is, therefore, a direct

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result of the rapid radiative association of CH_3^+ with H_2 to form CH_5^+. This process is also responsible for the predicted large abundance of CH_4. The evolutionary model results for CH_3CN and CH_3COH abundances can be reconciled with their observed values by simply adjusting the relevant radiative association reaction rate constants. The predicted CH_4 abundance will, however, remain large because we used the measured rate constant of the $CH_3^+ + H_2 \rightarrow CH_5^+ + h\nu$ reaction. The use of T = 50K in the equilibrium model drives the abundances of CH_3CN and CH_3COH in the right direction (although by too much) by suppressing the radiative association of CH_3^+ to form CH_5^+. (The high CH_3OH abundance in the warmer equilibrium model should not worry us, considering the very large abundance of water in the equilibrium models which did not allow water to condense onto the grains.) Temperatures on the order of 20-25K, rather than 10K, in the core of the dark clouds will, therefore, also bring about a better over all agreement between the predicted and the observed abundances. Compared to the tuning of several reaction rate constants, a slight change in just the temperature only is an elegant alternative. However, temperatures on the order of 20-25K in the cores of dense clouds, where the density may exceed $10^5 cm^{-3}$, may present problem for the heat budget in our model clouds with no internal heat source. Ion-neutral drift decreases the rate constants of three body association reactions (35). For clouds with magnetic fields, therefore, we have the third possibility that ion-neutral drift due to ambipolar diffusion may suppress radiative associations if the additional center-of-mass energy is equivalent to a higher "effective" temperature. This possibility too has its own share of problems due to uncertainties in the factors governing the magnitude of the ion-neutral drift velocity. These factors include the strength of the magnetic field, fractional ionization, and their dependence on the density (36). On the plus side the magnetic fields have the attraction that they help in slowing down the collapse.

7. FUTURE PLANS

Given the present results, it is now necessary to examine the slower collapse on a physically realistic basis by introducing magnetic fields. Another enticing question is the evolution of a cloud which experienced a significant shock compression and the associated chemical changes while it was still diffuse and was evolving very slowly towards its final dense state. We plan to explore these issues. CO self-shielding (37), *ab initio* calculation of the temperature, and a better estimate of the internal uv radiation field will be included in our future studies.

8. SUMMARY

The goal of evolutionary models of interstellar chemistry was defined to include the determination of the way in which clouds became what they are, the prediction of how they will change with time, and the

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investigation of the evolutionary sequence between these clouds and related heavenly bodies such as stars. We then presented an improved Mark II model of chemistry in dynamically evolving interstellar clouds. Results from the Mark II model indicate that the observed abundances of CI and CO and the non-detection of O_2 in dense interstellar clouds can be modeled with the conventional C/O < 1. Purely dynamical models of cloud evolution do not generate adequate observable discriminators of the predicted tracks. Coupled chemical-dynamical models have the exciting potential to yield useful supplementary diagnostics of the dynamical evolution.

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DISCUSSION

HARTQUIST: I find work like this is useful, because it demonstrates the way in which the chemistry evolves on time scales which probably characterise the dynamics in clouds. However, the many existing models of chemistry in collapsing clouds fail to take account of the probable importance of absorption onto grains and the lifetime of clouds, which survive far longer than the collapse timescales in the models.

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Chemistry in realistic dynamical models must be considered. Boland and de Jong have made a model of the chemistry in a dynamic but long lived cloud as have Williams and Hartquist; in both cases, grain absorption was considered. Much more work on the dynamics and the chemistry of long lived clouds is necessary.
PRASAD: I agree that much more work needs to be done on the dynamics and chemistry of long lived clouds. We are trying to do just that.

D'HENDECOURT: Solid CO on grains has indeed been observed in a few embedded IR sources, showing that CO will stick onto the grains, just as H_2O. Moreover, on the grains, CO can easily be converted to CO_2 which cannot yet be observed. So the amount of C in CO (and may be CO_2) is probably comparable to the amount of C in CO gas phase. Is it justified to consider only the sticking H_2O, neglecting that of other species?
PRASAD: Rigorously, it is certainly not justified to consider the sticking of H_2O only while neglecting the sticking of all other species, such as CO. However, while CO is observed in even dense clouds, water is not. Assuming that non-detection of water is not an excitation problem, i.e., if the non-detection of water is mostly due to its very low abundance, the above would suggest that there is something special about water which may justify our provisional assumptions.

GREENBERG: I should like to express my thanks to Dr. Prasad for making this first effort to understand cloud chemistry and cloud evolution as inseparable physical phenomena. As you know I have been exposing for years the concept of grain evolution intimately related to cloud evolution. One aspect of this, which we have developed (Tielens and then d'Hendecourt) is the role of grain in the cloud chemistry via surface reactions and explosion. I think it is time we tried to bring these two aspects together in a coherent scheme. It should not be necessary to have H_2O accretion on grains as a "black box" assumption when there is a ready made solution in terms of time dependent chemistry of grains and gas (d'Hendecourt, Allamandola and Greenberg A & A 1985).

TURNER: In the types of clouds you model, especially at the lower temperatures, the properties are those of "cold dark clouds" in which OH is a well studied species with reliably determined abundances (10^{-7} to 10^{-6}). Since $OH + O \rightarrow O_2$ is a key pathway in your scheme, OH must be a key constraint in predicting O_2 and CO abundances ($C + OH \rightarrow CO + H$ for the latter). Are the observed OH abundances consistent with your predictions for O_2 and C/CO abundances?
PRASAD: We can get the abundance of OH ~ 10^{-6} very easily but this disturbs both the C and O abundances. But one can control both these situations by introducting some activation energy in the reaction of C with OH.

FEDERMAN: Two comments are in order regarding Barry Turner's discussion on OH. First, the radio data probably sample gas with A_V equal or less than 5 mag, and thus cannot be used to analyse the cores of dense clouds. Second, CI has not been observed in cold clouds because of excitation conditions.

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TURNER: The radio lines of OH in dark clouds are demonstrably optically thin (hyperfine ratio). Therefore no optical depth effects prevent sampling the cloud cores in OH. Additionally, maps of such clouds by telescopes of greatly differing spatial resolutions give result suggesting that OH is not confined to outer regions (halos). If it were confined thinly, some indications of shell structure, easy to interpret because of the optical thinness, would have been observed.

PANDE: It is very interesting to note that dynamically evolving cloud models are being made. Is it not necessary to couple the hydrodynamic equations with radiative transfer equations for deriving true molecular abundances, if the situation is not fully represented by an optically thin case?
PRASAD: Yes, ideally we should treat radiative transfer and hydrodynamics jointly. Gerola and Glassgold's study (Ap.J. Suppl., 37, 1, 1978) is an example of such an attempt.

GUELIN: There are two evidences that CO is still abundant in the gas phase up to densities of 10^4 - 10^5 cm^{-3}, deep inside the dark clouds. The first comes from the CO/A_V or rather CO/A_{IR} - relation. We have reobserved with a much higher angular resolution (i.e. with the IRAM 30m telescope) the ^{13}CO and $C^{17}O$ column densities in the direction of a few highly reddened stars in Helies Cloud 2 (these stars were previously observed by Friberg, Langer and Wilson (Ap. J. 262, 590, 1982) with a low angular resolution). We find that, at least upto 10-12 mag of visual extinction, CO/A_V is not significantly smaller than in the region of the cloud where A_V = 2-5 (cf Guelin, this volume). The second evidence comes from the DCO^+/HCO^+ and N_2D^+/N_2H^+ abundance ratios. As the H_2D^+ recombination rate is small (cf. Smith and Adams, this volume), the deuterium enhancement in H_3^+ (and probably that in HCO^+ and N_2H^+) is calculated by the CO abundance. Then we derive $x(CO) \cong 10^{-4}$ similar to that found in the less dense parts of the clouds. These points are presented in more detail in a paper in preparation by us (to be submitted to Astronomy and Astrophysics).

IRVINE: As an observer, I would urge caution to the theoreticians in accepting published estimates of abundances too literally. These are very difficult determinations. Although some values are known reasonably well, others are quite uncertain; i.e., C_3H has been found only in one cloud (TMC-1); although C_2H_2 is widely distributed, its abundance has not been accurately determined in any specific cloud. Moreover, abundances for some species do differ among clouds which appear to be similar physically (i.e., the cyanopolyynes in TMC-1 and L183). Can such physically similar clouds be at different stages of evolution?
PRASAD: Your remarks about exercising caution in the use of the published observational abundances is certainly well taken. The possibility that clouds reaching almost similar physical conditions via different evolutionary tracks may have substantial chemical differences has been one of the motivations for evolutionary models. Theoretical modelling

results, however, are not secure enough at this time to make a definitive judgement on the possibility.

JACKSON: Regarding grain chemistry, one has to recognize the extreme difficulty in really knowing what the rate coefficients are on the grain. Experimentalists, interested in gas-surface reaction rates, spend half a million dollar building very elaborate apparatus so that they can ensure that surface is clean to know what the characteristics of the surface are, what kinds of defects are there on the surface and what not, none of which are known in the interstellar chemistry. As Bill Irvine points out, the observational exactness of the numbers is really not known, and the rate coefficients for the gas and surface reactions are not known. So, one has a situation where there are a large number of unknown parameters that one is trying to model. So what do we expect to get out of the model? What we expect to get is to learn how to handle these kinds of equations. Everybody sitting down here are agreeing about the details of your models without worrying about whether the model makes sense or not. The purpose of these models is not to know column densities and other details but to provide an experience in putting all the things together so that as one gets more and more accurate data from laboratory and observations, one can hope to put it together in a reasonable model.
PRASAD: Yes, we modellers do try to work in concert with laboratory workers and with observers to define the observational as well as laboratory strategy. It is after all an interactive process.

P.K. GHOSH: Besides the numerical values of final concentrations of the chemical species resulting from the model, it would be desirable if weightage of the various chemical processes that contribute to final concentrations are examined. This has the advantage of distinguishing major constituent chemical processes, and if the rate coefficients of such processes are not experimentally obtained, it would indicate reactions where experimental studies are crucially needed.
PRASAD: I agree. You have made a practical point. In the past we have tried to identify the major production and loss mechanisms at any particular epoch of evolution. We shall continue to do that.