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**Models of molecular clouds**

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## ABSTRACT

In this thesis I present the results of numerical model calculations of molecular clouds. The objective of this work is to study processes leading to star formation. The cloud models are calculated by solving simultaneously the equations of hydrostatic equilibrium, of thermal balance and of chemical equilibrium. In chapter IA I adopted as a representation of a molecular cloud a plane-parallel hydrostatic layer supported by turbulent pressure. In chapter IB I have constructed self-gravitating models of molecular clouds which are supported by turbulent and thermal pressure. The results show that all models are strongly centrally condensed. This fact has important implications for the distribution of the concentrations of several molecules. The gas temperature appears to decrease from about 40 to 80 K at the boundary of the cloud to about 10 K in the dense interior where  $A_V > 3$ . The results further show that the fractional ionization of the gas varies from  $n(e)/n_H = 10^{-4}$  in the outer layers of the cloud to about  $10^{-8}$  in the centre. This fact may have important implications for the role of magnetic fields in relation to star formation.

The plane-parallel models constructed in chapter IA satisfactorily reproduce the column densities of several molecules observed in the direction of the dust cloud L134. One of the novel aspects of these model calculations is that I included the fact that heavy elements condense on grains at the typical densities and temperatures that prevail in molecular cloud cores. To account for the observed C, N and O abundances in the centres of these clouds I had to postulate that molecular clouds are younger than  $10^6$  yr or that the condensation process is inefficient. Both possibilities are improbable and therefore unattractive. To resolve this problem I suppose in chapter II that matter in molecular clouds is circulating by turbulent motions such that continuously undepleted matter from the outer layers of the cloud returns to the core. At the time strongly depleted matter reaches the envelope of the clouds of a second time the grain mantles will be completely photodesorbed by interstellar ultraviolet photons or evaporated by an optical light flash of a nearby supernova. This circulation model is attractive to solve the depletion problem because the condensation time is of the same order of magnitude as the circulation time if the matter flows with a velocity approximately equal to the local sound speed.

In chapter IB I have constructed an improved cloud model including the proposed circulation prescription. In contrast with the plane-parallel models these improved models show a definite core-halo structure due to their spherical geometry. These models give a good fit to the column densities and the line intensities of more than ten molecules observed in L134, L183 and TMC-1. They predict a C/CO column density ratio of order unity in agreement with recent CI observations. It appears that the atomic carbon is predominantly located in the outer parts of the cloud ( $A_V < 2$ ) while the CO is predominantly in the core. The fact that the time required to convert atomic C to CO is of the same order of magnitude as the circulation time only slightly affect the predicted C/CO column density ratio.

In chapter IC I have calculated the chemical rate equations and the depletion time-dependently for one of the models presented in chapter IB. It appears that in the outer layers of the cloud (where photoreactions are important) most species are in chemical equilibrium. Therefore the predicted column densities are only slightly affected by the time-dependent treatment of the chemistry for those species that are predominantly located in the outer parts of the cloud. In the cloud core the abundances of saturated molecules like  $C_2H_2$ ,  $CH_4$ ,  $H_2CO$ ,  $O_2$  and  $N_2$  and of  $HC_3N$  differ significant from the equilibrium concentrations. Because these molecules are located exclusively in the dense interior of the cloud also their column densities differ strongly from those reported in chapter IB. Our circulation model can only account for the observed  $HC_3N$  column densities if the chemistry is calculated time-dependently.

It is shown in chapter III that the  $l_{10}$ - $l_{11}$  transition of formaldehyde can be inverted by the free-free continuum radiation of an ultra-compact HII region. Based on the proposed pump mechanism a model is presented for the formaldehyde maser near NGC 7538 - IRS 1. Formaldehyde masers appear to be exceptional because the 6 cm transition of  $H_2CO$  is observed in absorption towards several other compact HII regions associated with OH maser emission. It is argued in chapter IV that these HII regions are surrounded by dense neutral material so that the lower rotational lines of formaldehyde are thermalized.