Abstract

The components of the interstellar medium (ISM) are continuously heated due to energy input from different sources, one being the radiation of young and massive stars. In photon-dominated regions (PDRs) the interstellar far-ultraviolet (FUV; 6-13.6 eV) radiation field determines the energy balance and the chemistry of the ISM. Consequently, PDRs form in different astrophysical scenarios, for instance at the edges of irradiated molecular clouds. Depending on the cloud's characteristics, stars may form from dense, embedded cores. To understand the interaction between FUV radiation and star formation it is necessary to gain detailed knowledge of the physical conditions and the intrinsic structure of the ISM in molecular clouds and PDRs.

Cooling of the gas in PDRs is dominated by fine structure line emission by atoms and ions, as well as rotational and vibrational line emission by molecules. The KOSMA-τ PDR model simulates the chemical and physical structure and the line emission of spherical clouds ("clumps") in the ISM.

In this thesis the KOSMA-τ PDR code is used to simulate transitions from atomic to molecular hydrogen ("HI-to-H_2 transition"). The characteristics of these transitions are governed by the parameter αG, which depends on the ratio between FUV flux at the cloud surface and cloud density. Numerically derived properties of the clumps, like their HI column densities or H_2 mass fractions, are compared to analytic formulae provided by Sternberg et al. (2014) as well as to results from McKee & Krumholz (2010). A generalised definition of critical clumps is proposed, where, for a fixed αG but varying clump size, the critical clump provides the largest HI column density between its centre and surface. The numerical results closely follow the analytic formulae and support the generalised definition of critical. Small inaccuracies remain for small αG.

Observations suggest that the ISM can be modelled using fractal structures. Furthermore, it has been shown that a superposition of spherical clumps, having a specific mass-spectrum and a specific mass-size relation, can be used to mimic the structure of the ISM. The resulting ensemble of dense clumps is generally found to be embedded into a thinner interclump medium.

In this thesis, I introduce an extension of the KOSMA-τ code, denoted KOSMA-τ 3D, which can be used to model star forming regions with arbitrary three-dimensional (3D) geometry. In this model, a 3D compound made of voxels ("3D pixels"), containing ensembles of clumps with discrete mass distributions, is generated. The characteristics defining the ensembles can vary between different voxels. A probabilistic approach is used to calculate the averaged FUV extinction caused by the clumps within each voxel. To analyse each individual clump the new code is combined with the KOSMA-τ

PDR model. Line intensities and optical depths of individual clumps are used to calculate the distribution of voxel-averaged intensities and optical depths, and the radiative transfer through the compound yields full spectral cubes. Thereby, the new code accounts for the intrinsic linewidths of single clumps and additionally for a velocity dispersion of the clump ensemble.

The Orion Bar PDR, a well-known and luminous star forming region with an interesting edge-on geometry, is used as a test-case for the new 3D code. New HIFI/*Herschel* data from the HEXOS guaranteed-time key program and complementary data from the *Caltech Submillimeter Observatory* (CSO) are fitted.

Furthermore, I present simulation results, based on the clumpy edge-on cavity wall suggested by Hogerheijde et al. (1995) and on a cylindrical filament geometry. Simulations and observations are compared in terms of the layered positions of the emission peaks, the "chemical stratification", and the line integrated intensities at the peak positions. Most PDR models fail to reproduce this combination.

Analysis of different models shows that in the cavity wall, a large fraction of the total mass needs to be contained in clumps. The characteristics of the interclump medium are constrained by the depth of the FUV penetration. Furthermore, the stratification profile cannot be reproduced by a model having the same amount of clump and interclump mass in each voxel, but dense clumps need to be removed from the PDR surface. Also, the number of voxels along the line of sight into the direction of the observer at the inner edge of the cavity wall must not be significantly smaller than along other lines of sight, deeper in the cloud. Therefore, strongly inclined cavity walls or the cylindrical geometry fail. The best fitting model reproduces the line integrated intensities of many simulated cooling lines within a factor four and the stratification pattern within 0.02 pc (or better).