Theory Meets Observations

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PDRs are formed wherever FUV radiation illuminates the surface of molecular clouds and as such make up a significant part of the observable ISM in galaxies ("PDRs are everywhere"). Therefore, PDR models play an important role in the interpretation of ISM observations. Existing and future observatories specifically target the wavelength regime where much of the PDR dust continuum and line radiation is emitted. Examples are the Spitzer Space Observatory, the Stratospheric Observatory for Far Infrared Astronomy (SOFIA) and the Herschel Space Observatory. Together, they cover the spectrum from NIR to (sub-)mm wavelengths. They allow observations of warm dust emission from FUV-heated dust and PAH particles as well as the principle gas cooling transitions including H_2, CO and the fine-structure transitions of neutral and ionized carbon and neutral oxygen. Moreover, the ground-state transition of many hydrides are accessible by these air and space-borne observatories, providing a relatively complete inventory of chemical species in PDRs. Ground-based (sub-)mm observations with the SMA and ALMA interferometers provide better angular resolution and thus an opportunity to study the small-scale spatial structure (clumpiness) in PDRs. Together, these observations will provide new challenges for PDR simulations.

Large ongoing and future mapping projects of the ISM such as the surveys made of the Galactic Ring and the Cyg-X region at various wavelengths, on the other hand, call for a method to quickly assess the physical parameters and chemical composition of the gas. Furthermore, it might be possible to use PDR simulations for the interpretation of observations of tracers which are not primarily thought to be PDR tracers, but which are emitted in regions where the physics and chemistry is governed by an external FUV field. Examples are HI surveys of galaxies in combination with the known metallicity and newer, more accurate measurements of the FUV field which will be available with the Galaxy Evolution Explorer, GALEX. This expands the applicability of PDR models and at the same time tests whether or not external FUV radiation governs emission lines not thought to be classical PDR tracers. Such an application, however, might require the existing PDR codes to be modified. Finally, the increased use of existing literature and web publications of PDR models by observers suggests a strong interest in PDR simulations with easy-to-use interfaces.

Clearly, it is important to involve the observer community in the PDR benchmarking process. This could be in form of sessions in future workshops where specific modeling needs are discussed and how these needs could be met with current PDR models. These discussions could provide guidance for the PDR benchmarking effort by identifying tracers and defining the PDR parameter space where future PDR simulations are desirable. However, it is generally agreed that a wider observer community should be involved only after the current first round of iterations and thus after the larger differences between the individual model results are corrected or better understood.

From an observer point of view it is attractive to have PDR simulations available in the form of an automated tool box where physical parameters (for example, density) can be derived for a given set of observations (line intensities, line ratios and abundances). This results from the sheer number of observations and from the fact that only a fraction of the observing community has immediate access to PDR codes and expertise. Along with the PDR models, the accuracy and the limits of applicability should be communicated. In this context a simple definition of a PDR model is helpful, as well as some general remarks regarding known limitations. A test might be provided which can be used to decide whether the chemistry and line excitation of the region under consideration indeed is governed by a PDR, or if other processes have to be considered and where a "PDR-only" approach will likely fail. For example, tracers where a modeling in the framework of a PDR is known to be difficult (eg. CH^+ in diffuse clouds) and tracers which are sensitive to shocks (for example, H_2O transitions, and mid- and high-J CO transitions).

To summarize, PDR model simulations provided within a tool box should be accompanied by additional information on

- the assumptions and approximations used in the model, together with the PDR parameters defining the limits of application of the PDR model results, and
- the accuracy which can be expected from the PDR model calculations, given the uncertainty in the parameters, observations and model assumptions.

Listing critical model parameters is of particular importance. These are parameters which are relatively poorly known but might have a substantial impact on the PDR model results. One example discussed during the workshop is the initial abundance of sulfur and PAHs and the implication for the neutral carbon abundance profile throughout the model cloud. Here, the benchmarking models of the Leiden workshop are particularly useful, even if they narrow the scope of PDR models. These models can be used to identify critical parameters, quantify the uncertainty of the model results as a function of the approximations used, and trace the impact of future updates of the PDR model parameters (abundances, chemical rates and collision rates) due to newer and better measurements and calculations. This provides the observer with a guideline on what PDR models can deliver. In this context, it is desirable to add a limited number of observed clouds as benchmarking models. Preferably, these are clouds/regions which are well studied by observations and where the physical parameters are relatively well known.