Comparing Reduced Vs. Full Chemical Networks

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Introduction

Molecular clouds are giant compounds of cold gas and dust. These clouds are home to young forming stars. Understanding their chemical composition is a crucial part in the study of star formation. However, due to computational expense, many chemical studies use reduced models of chemical networks that contain only tens of reactions, neglecting many key species. Comparing results from three different chemical networks helps to answer the question "***How accurate are reduced networks compared to full ones?***" The three networks which will be implemented are: Nelson and Langer (1999), Glover et. al. (2010), and the UMIST database (Miller et. al., 2022).

Network	Number of Reactions	Number of Chemical Species
Nelson and Langer	23	14
Glover	219	32
UMIST	6173	468

Methods

Given a physical state, a list of chemical species, and reactions between these species, we can model the time evolution of the abundances of these species. The i'th rate of change of concentration for a given species is given by:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \sum_{j \in F_i} \left(k_j \prod_{r \in R_j} n_r \right) - \sum_{j \in D_i} \left(k_j \prod_{r \in R_j} n_r \right)$$

where n_i is the species, F_i is the set of reactions in which the i^{th} species is being formed, k_j is the reaction rate of the j^{th} reaction, R_j is the set of reactants for the j^{th} reaction, and D_i is the set of reactions where the i^{th} species is being destructed. This creates a reaction system of Ordinary Differential Equations to be solved in Julia using the OrdinaryDiffeq.jl package.

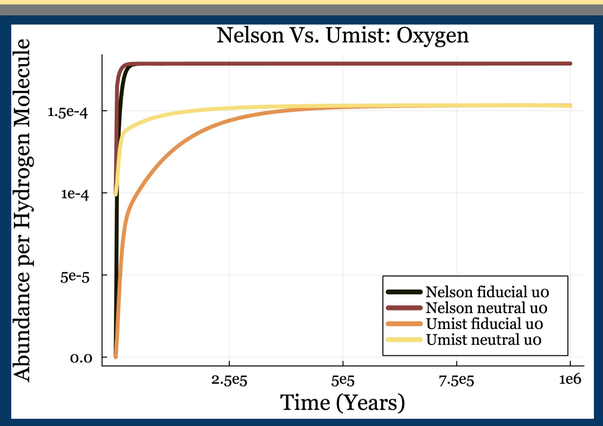
The Nelson, Glover, and UMIST networks will be solved with the same initial conditions and physical parameters and their results will be compared at 1 million years. This experiment also compares chemical outputs using two sets of initial conditions while conserving total abundance.

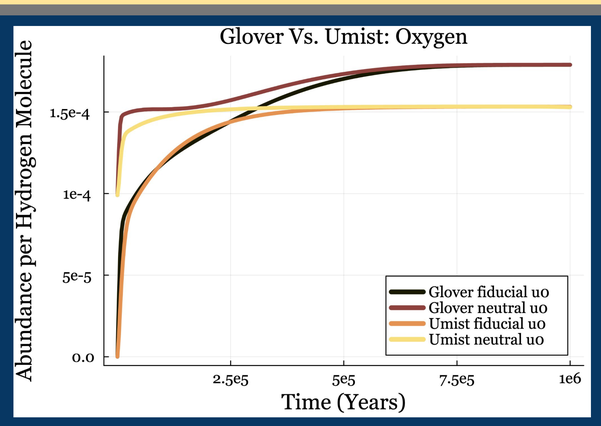
Results

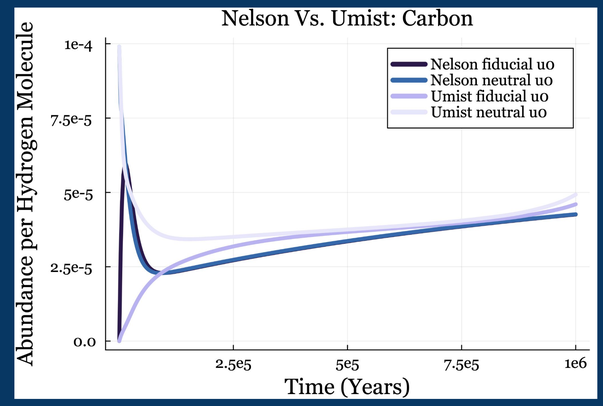
Figure 1: Abundance of Carbon (bottom row) and Oxygen (top row) per hydrogen nucleus versus time.All models use the same physical parameters:

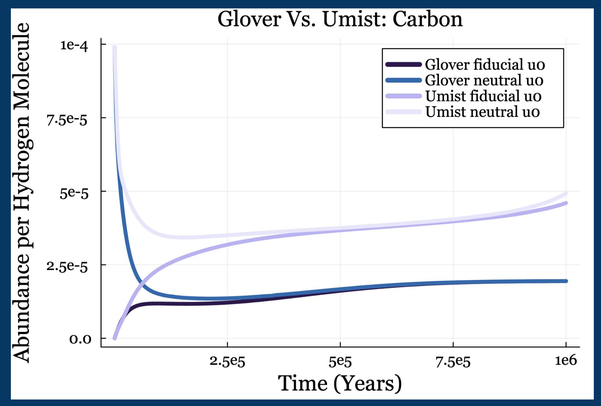
- ★ Temperature = 300 kelvin
- ★ Visual Extinction Av = 2 magnitudes
- ★ G0 = 1.7 (solar neighborhood radiation)
- ★ Number Density = 611 cm^{-3}
- ★ Cosmic ray ionization rate = 6.18e-18 per second.

All networks were solved with two different sets of initial conditions (u0). First, "Fiducial u0" with initial values H_2 = 0.5, He = 0.1, C^+ = 1e-9, C = 5e-9, O = 1e-8, HCO^+ = 9e-9, CO = 9.9e-5, H_2O = 8e-5, O_2 = 1e-8, H_3^+ = 1e-8, and e = 0. Second, "Neutral u0" where initial abundances were changed but atom amounts were conserved with values H_2 = 0.5, He = 0.1, C^+ = 0.0, C = 9.91e-5, O = 1.79e-4, HCO^+ = 0.0, CO = 0.0, H_2O = 8e-5, O_2 = 1e-8, H_3^+ = 0.0, and e = 2e-8.









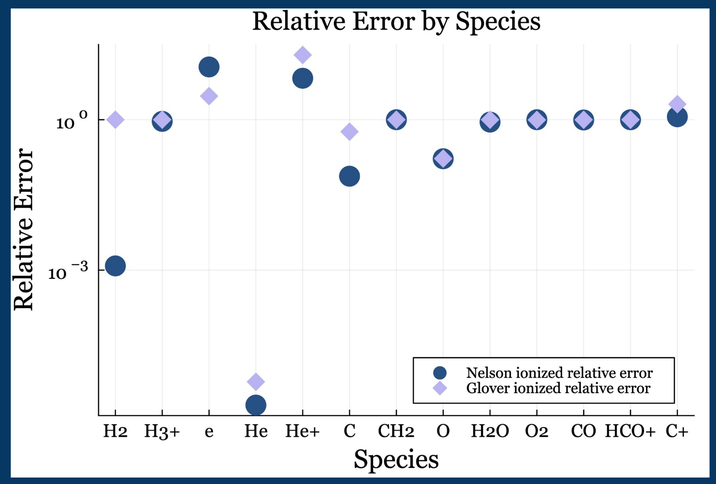


Figure 2: Relative error for the Nelson and Glover networks at time t = 1 million years with UMIST as the reference solution.

Conclusion

- Changing the initial conditions of a chemical network but conserving species will lead to the same steady state chemical output for that network.
- The Glover and Nelson networks produced similar relative errors to the UMIST network for typical molecular cloud conditions.

References and Acknowledgements

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