

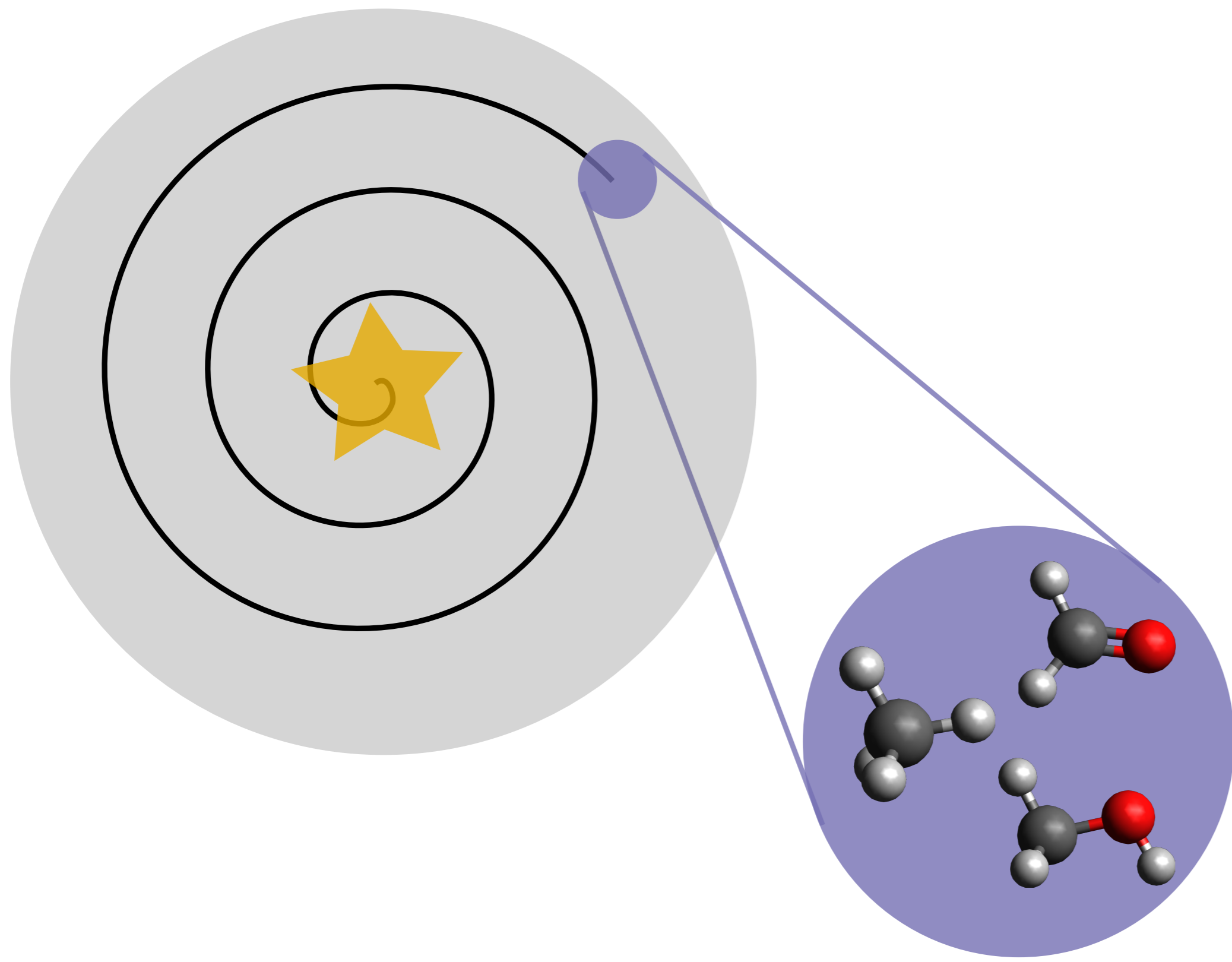
# Coupling Dynamics and Chemistry in Accreting Protoplanetary Disks

Ellen M. Price, L. Ilesedore Cleaves, and Karin I. Öberg  
Harvard-Smithsonian Center for Astrophysics



## BACKGROUND

Protoplanetary disks are complex systems of dust and gas orbiting young stars. Chemical reactions, both in the gas phase and on the surfaces of dust grains, determine which species become abundant and, therefore, which species will contribute to the initial compositions of forming planetesimals. Changes in physical conditions affect which chemical reactions can take place and how the disk evolves at a given radius. Many existing disk chemistry modeling codes compute the time-varying chemistry as a function of radius in the disk, but they do not take into account the changing physical conditions within the disk. Codes which do couple chemistry and dynamics are computationally expensive, preventing thorough exploration of parameter space. **This project takes a different approach by following local physical conditions in accretion streams of gas and small grains**, which should allow us to determine how parameters such as disk mass, disk viscosity, and stellar spectral type affect the underlying disk structure.



## METHODS

We modify an existing disk chemistry solver code (originally Fogel et al. 2011) by incorporating simple time-dependent physical parameters, such as temperature, based on analytic predictions for how physical conditions in the disk midplane evolve. The advantage of using a simpler code is that it will allow us to investigate, in detail, how different aspects of chemical evolution vary with different physical parameters. We begin with the self-similar disk surface density profile as an initial condition and assume that the disk viscosity can be described by the single parameter  $\alpha$ . We then solve the fluid equations to find the surface density as a function of time at all radii. From the surface density function, we derive a velocity field and, thereby, find an equation for the radial position of a parcel as a function of time and initial position. In Figure 1, we plot the evolution of several physical variables for a single parcel at various values of  $\beta$ , the power law index on the radial temperature profile ( $T \sim r^{-\beta}$ ) of the disk; for the rest of our analysis, we take  $\beta = 1/2$ . Other parameters we adopt are  $\alpha = 0.001$  and  $M_* = 1M_\odot$ .

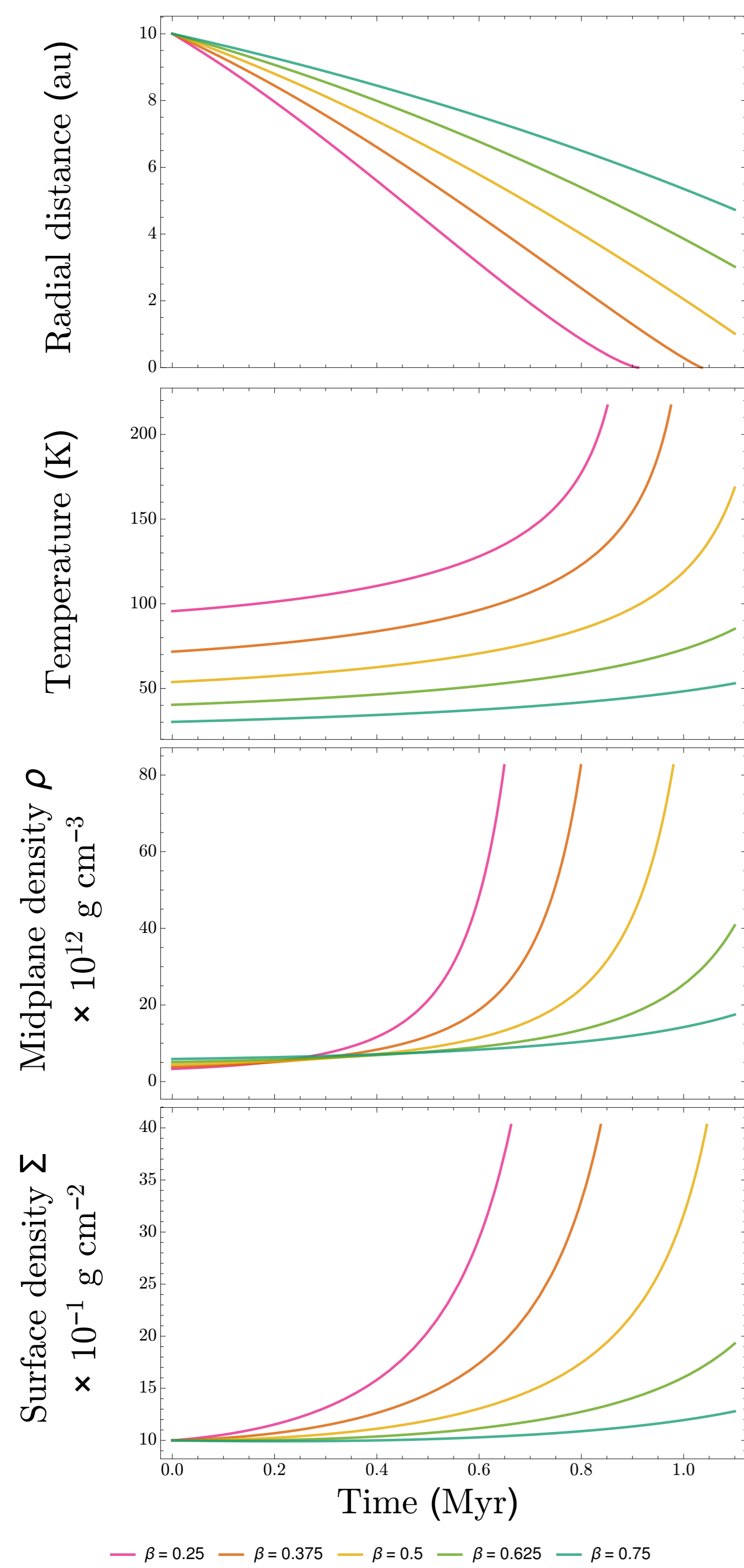


Figure 1: Time evolution of local physical properties of a gas parcel as it moves through the disk, assuming a starting position of 10 AU and nominal physical parameters described above.  $\beta$  is the temperature power law index, defined above.

## RESULTS

Our results are the product of two simulations. In one simulation, the physical variables are varied as described above; we will refer to this simulation as the “dynamic case.” In the second, “static,” case we hold the parcel fixed at the endpoint of the dynamic track for the entire simulation. **We show that bringing a gas parcel in from larger radii (and lower temperature) overproduces hydrocarbon chains compared to the static case.** This could help explain observations such as Kastner et al. (2015) and Bergin et al. (2016).

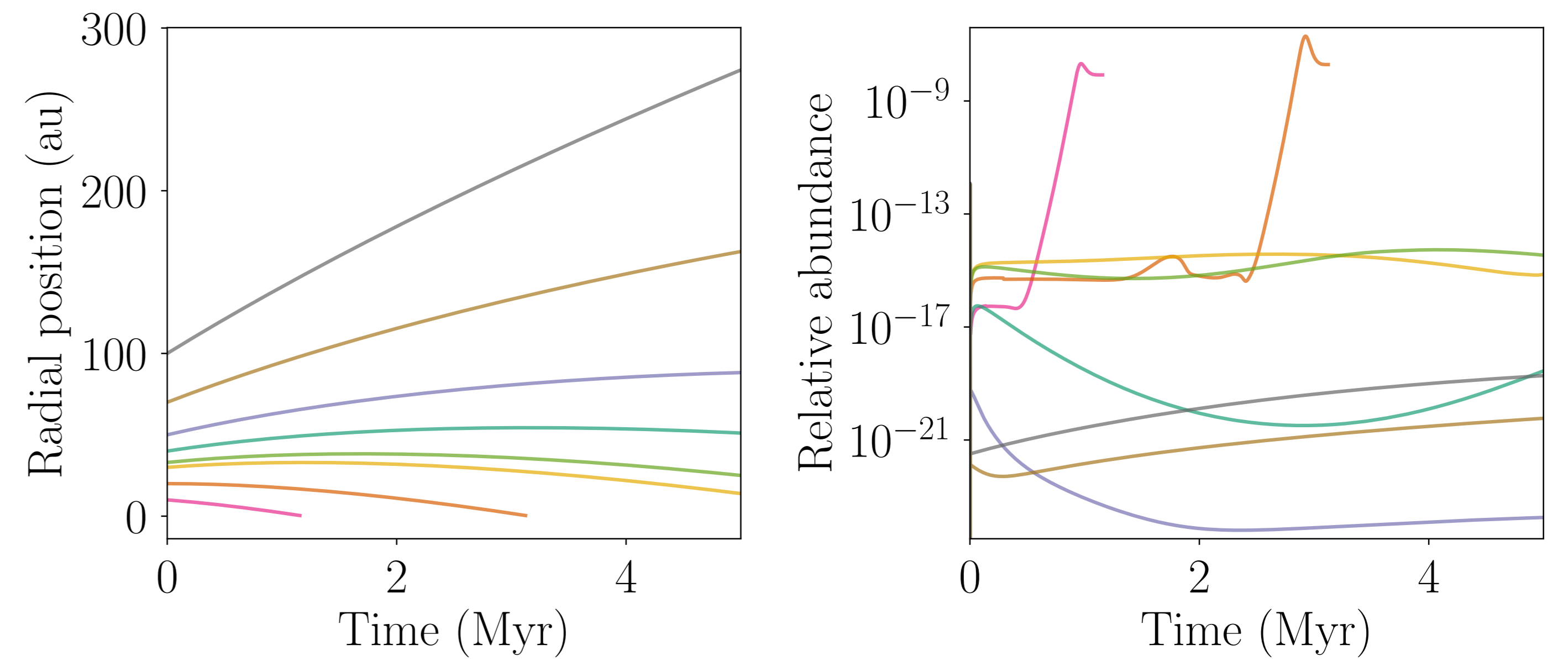


Figure 2: For a variety of tracks through the disk, we follow the chemistry of  $C_3H$  as a function of time and observe a variety of behaviors.

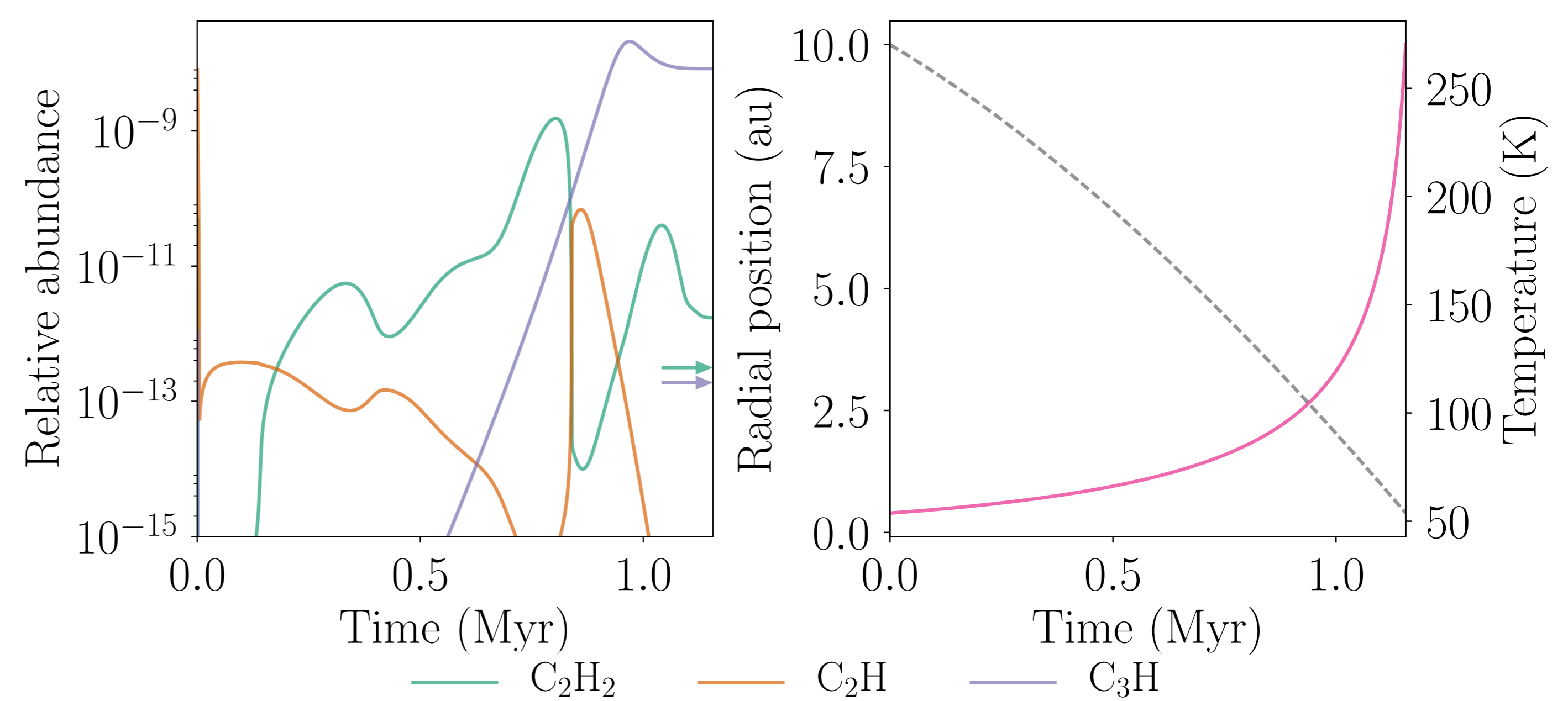


Figure 3: For a single track that begins at 10 AU, we follow the chemistry of  $C_2H_2$ ,  $C_2H$ , and  $C_3H$  as a function of time. Arrows indicate the ending abundances of the corresponding static simulation.

## SUMMARY

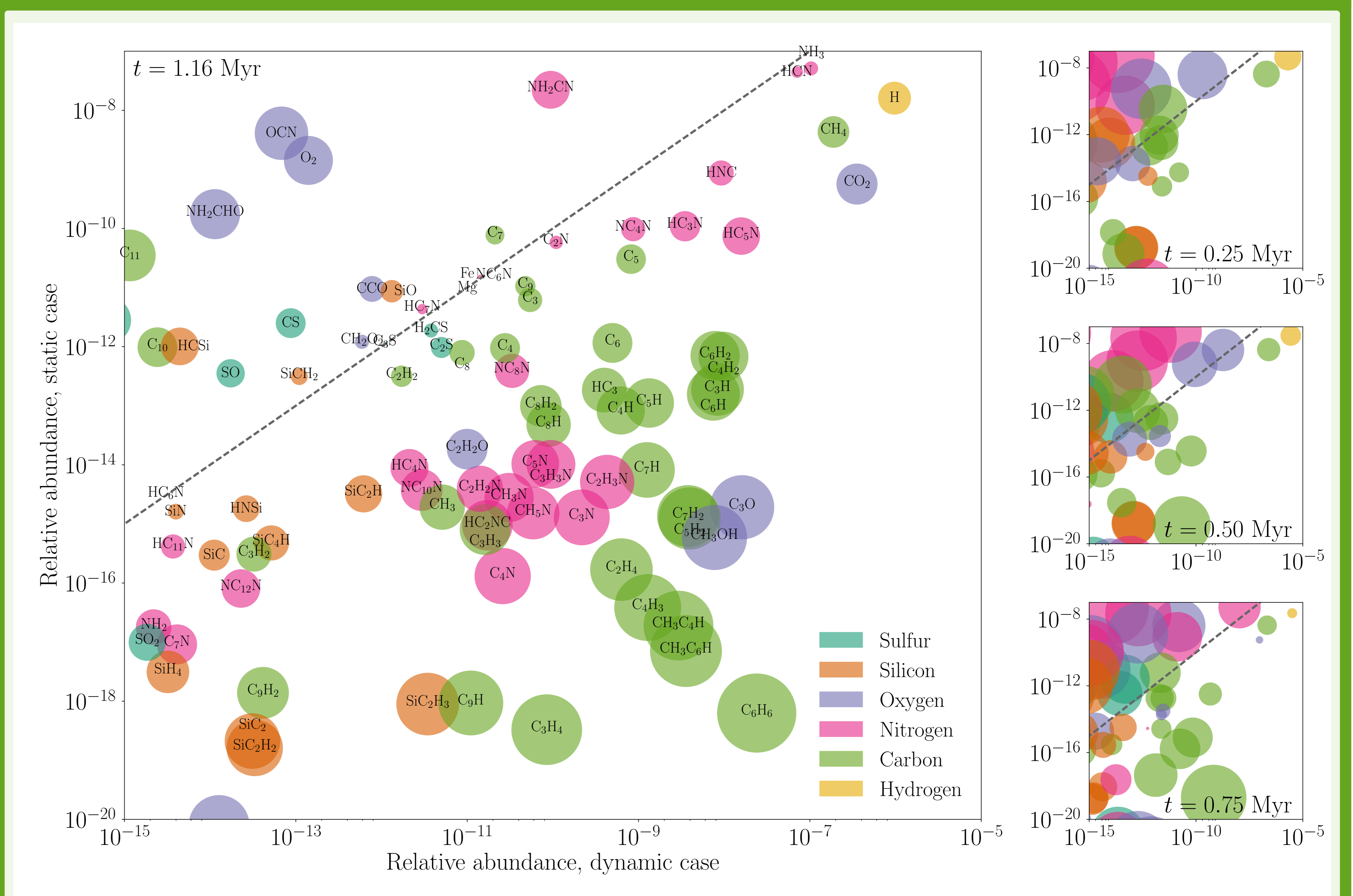


Figure 4: Relative abundances in the static case vs. in the dynamic case. The dashed line indicates where the two relative abundances are equal; deviations from this line indicate that the dynamic case under- or over-produces some species. Circles indicate different species, colored by the heaviest atom; the size of each circle is related to the logarithm of the maximum ratio of the absolute abundances, a measure of how “important” each species is in the model.

## REFERENCES

Bergin, E. A., Du, F., Cleaves, L. I., et al. 2016, ApJ, 831, 101  
Fogel, J. K. J., Bethell, T. J., Bergin, E. A., Calvet, N., & Semenov, D. 2011, ApJ, 726, 29  
Kastner, J. H., Qi, C., Gorti, U., et al. 2015, ApJ, 806, 75

## ACKNOWLEDGEMENTS

EMP gratefully acknowledges support from the National Science Foundation through a Graduate Research Fellowship and funding from the Harvard University Astronomy Department’s Pierce Fellowship.