Semi-analytical solutions perform well against complex calculations involving condensation (solid phases)

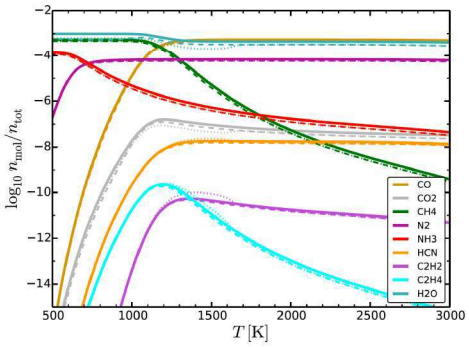


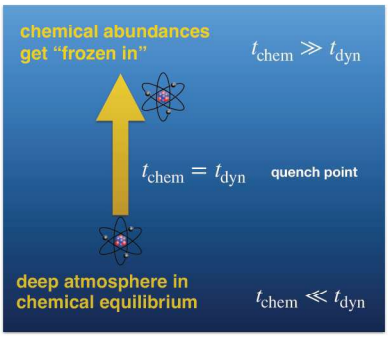
Fig. 4. Concentrations of major molecules at 1 bar according to a simplified nine-molecule model in chemical equilibrium (full lines), in comparison to a model with 24 elements and 445 molecules (dashed) and a full model with equilibrium condensation (dotted).

Woitke et al. (2018, A&A, 614, A1)

How do we make calculations when $t_{\rm chem} \gtrsim t_{\rm dyn}$?

1. Quenching approximation
2. Chemical kinetics

Computing disequilibrium chemistry: quenching approximation

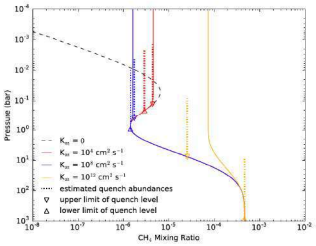


We may develop intuition about disequilibrium chemistry as a non-local problem associated with transport

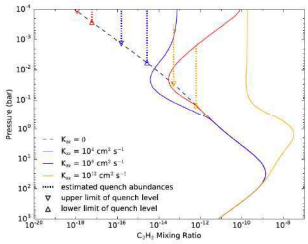
e.g. CO observed in Jupiter
(Prinn & Barshay 1977, Science, 198, 1031)

Why the quenching approximation lacks generality

$$t_{\rm dyn} = \frac{K_{zz}}{L^2} \longleftarrow L \sim 0.1H \text{ to } H$$



methane is controlled by transport-induced quenching



acetylene is not… it is instead controlled by disequilibrium abundance of methane

Tsai et al. (2017, ApJS, 228, 20)

Equations of chemical kinetics

$$\frac{\partial n_i}{\partial t} = \mathscr{P}_i - \mathscr{L}_i + K_{zz}\frac{\partial^2 n_i}{\partial z^2}$$

loss term

production term

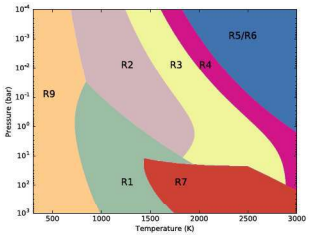
atmospheric mixing in 1D (approximated as diffusion)

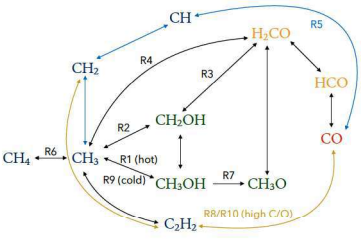
One needs to account for every species *i* in the chemical network, which includes transient species.

Typically, each chemical network contains hundreds, if not thousands, of reactions.

Pretend that advection, convection, turbulence, etc, may be described by some global diffusion coefficient.

Example: part of a chemical network to convert methane to carbon monoxide





The rate-limiting reaction is the slowest reaction in the fastest pathway.

But it depends sensitively on temperature and pressure!

Tsai et al. (2018, ApJ, 862, 31)