Chiang & Goldreich (1997)

* derive hydrostatic, radiative equilibrium models for passive disks around T Tauri stars
* assume flared disk rather than flat
* calculate the SED for the passive disk self consistently
* first assume blackbody disk
* for flat disk T\_e ~ a^(-3/4)
* hydrostatic equilibrium => flared disk
* then, drop blackbody assumption and determine the SED through radiative transfer
* assume that gas and dust temperatures are equal in the interior
* first consider flat disk, then flared
* compare with observations => the SED of GM Aur is consistent with a passive reprocessing disk

D’Alessio et al. (1998)

* accretion disk around T Tauri star taking into account accretional heating
* assume gas and dust in disk are well mixed and thermally coupled; disk receives radiation from the central star and through viscous dissipation, cosmic rays and radioactive decay
* energy transport through turbulent flux, radiation, convection
* steady state, disk geometrically thin, hydrostatic balance
* results for their fiducial model:
  + disk is optically thick to stellar radiation, but may be optically thin to its own radiation
  + temperature: for a < 5 AU, flaring not important => T ~ a^(-3/4) as in an irradiated flat disk
  + viscous dissipation is the main energy source for a < 2 AU
  + there is a disk atmosphere; there is also a temperature inversion due to stellar radiation
  + main improvement of this model is that they calculate the optical depth self-consistently rather than assume that the disk interior is optically thick
  + surface density consistent with analytic predictions
  + disk mass, timescales calculation
  + energy transport: convection only important in the midplane at a < 0.01 AU
  + gravitational stability: nonirradiated disk more likely to become gravitationally unstable at large a than irradiated disk

D’Alessio et al. (1999)

* use the disk model of D’Alessio et al. (1998) to explore how disk structure varies with alpha and Mdot
* compare with observations => models can explain near IR fluxed of T Tauri stars for disk accretion rates consistent with mean value estimates
* however, models seem to be too geometrically thick at large radii => dust settling could substantially reduce the geometric thickness of the disk => explore this in subsequent paper

D’Alessio et al. (2001)

* disk structure including dust grain growth
* still assume complete mixing between dust and gas
* find that the resulting disk models are less geometrically thick than in the case where ISM opacities are used, and they agree better with observed SED distributions

**CHEMISTRY** Visser et al. (2009)

* aim: understand how material changes chemically as it is transported from the molecular cloud to the star and the disk
* model the chemical evolution from the pre-stellar core to the disk phase in 2 D using a simplified semi-analytic model
* gas and dust are expected to be well-coupled => gas and dust temperatures are set to be equal
* the only chemical reactions they include are H20 and CO adsorption and desorption => total abundance of CO and H2O remains constant in each parcel
* CO and H2O begin entirely in gas phase
* Model does not include radial and vertical mixing

Disk chemistry background for thesis proposal

* from Henning & Semenov (2013):
  + mention that complex disk chemistry models have been developed by several groups and cite some literature from Table 3
  + perhaps mention that these models have shown that chemistry in disks is mostly regulated by T, rho structure, stellar / interstellar radiation fields, cosmic rays
  + some background parts from the intro can be useful for my own intro
  + disk emission from CO in its rotational transitions can be often measured due to its relatively high abundance and permament dipole moment
  + time scales of key chemical processes have to be shorter than ~1Myr => reference to Semenov & Wiebe (2011)
  + see if there’s anything relevant to mention from Table 1 (i.e. about the observed emissions from any particular molecule, perhaps from CO would be relevant)
  + abundances of discovered molecules range between ~10^-10 – 10^-4 relative to H2
  + observations find depletion of molecules relative to molecular abundances in the ISM -> caused by freeze-out or photodissociation in the disk atmosphere
  + detection of molecular ices => look at Aikawa et al. (2012, A&A 538, A57)
  + PPD’s have strong vertical and radial T and rho gradients + different radiation fields at various disk locations => diverse disk chemistry -> see summary of reactions in Table 2
    - inner disk <~ 20 AU: observed through IR spectroscopy
    - outer disk >~ 20 AU: observed through (sub)millimiter observations
  + chemistry approaches quasiequilibrium in inner disk due to high T and rho
  + for outer disk regions, high-energy radiation and cosmic rays are key drivers of chemistry; production of various ions
  + freeze-out of molecules at low T in the outer disk
  + chemical models:
    - early models: usually restricted to inner disk regions, 10-30 AU, thermodynamic equilibrium was usually assumed
  + chemical models of PPDs are based on detailed chemical kinetics models with hundreds or thousands chemical reactions => computationally intensive => decoupled from disk dynamics
  + more modern studies include various heating and cooling processes, plus grain evolution (refs 71, 98, 216, 260): 1D (ref 266), 2D approximation (ref42), X-ray radiative transport (refs 47, 52, 267, 268)
  + chemo-dynamical models: refs 207, 210, 273, 274, 275
  + more about chemistry coupled with dynamics models: Aikawa et al. (1999)… see if some references on page 9030 are worth mentioning
  + giant planets are believed to be formed outside the snowline, Kennedy & Kenyon (2008)
  + origin of water from Earth: delivered from comets, Morbidelli et al. (2010)

Semenov & Wiebe (2011)

* 2D model using the mixing-length approximation + time-dependent chemistry; for turbulent disk
* volatiles are preserved in comets
* paper about comets: Bradley (2005)
* when does turbulence affect chemistry?
  + Consider two timescales, t\_phys and t\_chem. If t\_phys < t\_chem, chemical evolution of a molecule is slow and thus sensitive to changes in the physical conditions; if t\_phys > t\_chem, chemical evolution and thus not affected by transport processes
  + Ion-molecule chemistry is very rapid, t <~ 10-1000 yr
  + Surface chemistry has a long timescale around midplane and in the outer cold regions, ~10^6 yr, larger than the turbulent mixing timescale

Cleeves et al. (2011)

* chemical model of a PPD with a large inner gap similar to those seen in classical transition disks
* radiation field: UV and X-rays; treatment of the radiative transfer in the disk
* reaction network: following Fogel et al. (2011); reaction types include photodesorption, photodissociation, freeze-out, grain surface reactions, ion and electron reactions, cosmic-ray and stellar X-ray ionization, radiative reactions

Bruderer et al. (2009), ApJS

* presents a method for the chemical modeling of young stellar objects, i.e. the chemistry changes / networks in between the cloud collapse phase and the formation of the protoplanetary disk
* consider heating due to FUV radiation and X-rays
* chemical reaction network; they interpolate abundances from a grid of physical parameters relevant for the chemical composition
* calculate reaction rates for photodissociation and ionization due to FUV radiation analytically (“classic” formulae)
* similarly for X-rays
* results for CO, CO2, H2O, etc. abundances in Fig. 4 (still for the collapse phase(?))
* main point: the grid of chemical models is publicly accessible (see website link at the beginning of section 5)
* look also at follow-up papers from 2009/2010

Bergin+15

* trace the evolution in the relative abundance of C and N from the ISM through planetary assembly => C/N ratio can provide clues into terrestrial planet formation and the delivery of volatiles to terrestrial planets
* ISM: gas-phase C/N lower than solar; interstellar ices have elevated C/N ratios (~12), but this doesn’t account for the presence of nitrogen as N or N2=> when these are taken into account, C/N ~ 1.8
* Comets have C/N ratios higher than solar (again likely due to the non-observability of N2)
* Earth: both surface reservoir and bulk silicate earth have C/N ratios higher than solar
  + => C/N increases from the ISM, to cold comet formation zones in the outer disk, to inner planetary nebulae, to planets
* mentions that nitrogen is primarily N2
* the main carriers of C in the inner solar system are organic ices and carbonaceous dust grains
* thermal evolution of small bodies derived from nebular dust and ice produced differentiated bodies with enhanced C/N ratios (?)

Du, Bergin + 15

* transition disks are expected to have an abundance decrease of C- and O- bearing species relative to dust due to the overall reduction of the gas mass; however, TWHya has a significantly larger observed mass than the mass inferred; this could be explained if the abundance of C- and O- bearing species are not depleted in the disk midplane and there may be an enhancement of their abundances in the inner disk; this implies that in the outer disk the main reservoir of volatiles resides in the disk midplane locked in solid bodies, and their migration to the inner disk can cause enhancements in C and O
* model assumes that only C and O are depleted differentially in the outer disk atmosphere, while nitrogen is left intact; consistent with observations of solar system ices / comets, which are nitrogen poor
* by depleting oxygen over the entire disk, the gas becomes rich in C and N bearing molecules, particularly inside the CO snowline

For Discussion:

* expect high both gas-phase and solid-phase N abundance in the outer disk => consistent e.g. with the nitrogen-dominated atmosphere of Titan at 10 AU

Our results for the N/O ratio in Section \ref{sec:N}

1. Comets are known to be depleted in nitrogen compared to the solar value, e.g. Halley by a factor of 2-6 (ref). The measured N2 abundance of comet 67P is a factor of ~25 lower than the solar abundance (ref); the low N2 abundance is consistent with the formation of comets inside the N2 snowline, but the presence of N2 also suggests a low formation temperature. Discuss here that the NH3 abundance in the solar system (and disks) is likely to be higher than the range observed in protostellar cores, since otherwise there would not be enough N-containing ices in the comet formation zone to explain their composition.
2. Our results are consistent with measurements of low C/N (i.e., high N/C) ratios in cold outer disk regions, as well as an increase in the absolute nitrogen abundance from the inner solar system to the outer nebula (Bergin+15). Our results are also consistent with high gas-phase N/O ratios in the outer disk. Based on mass measurements of transitions disk such as TWHya, theoretical models suggest that C and O bearing species are depleted in the disk upper layers, particularly beyond the CO snowline (Du, Bergin+15). Oxygen depletion, in particular, implies enhanced abundances of nitrogen bearing species in the outer disk and thus higher N/O ratios.
3. In the near future, observations of atmospheric spectra with instruments such as JWST are likely to provide constraints on C/N/O ratios in exoplanet atmospheres. Elevated N/O or N/C ratios in the atmosphere of a giant planet would suggest that the planet accreted its atmosphere in the cold outer disk regions, and thus these ratios may be used as tracers of the planet’s formation zone. It is thus crucial to build a quantitative theoretical framework to explore the range of gas-phase C/N/O ratios across disks with different dynamics and grain morphologies.