Astrochemical simulations：
星間化学モデルの現状と課題

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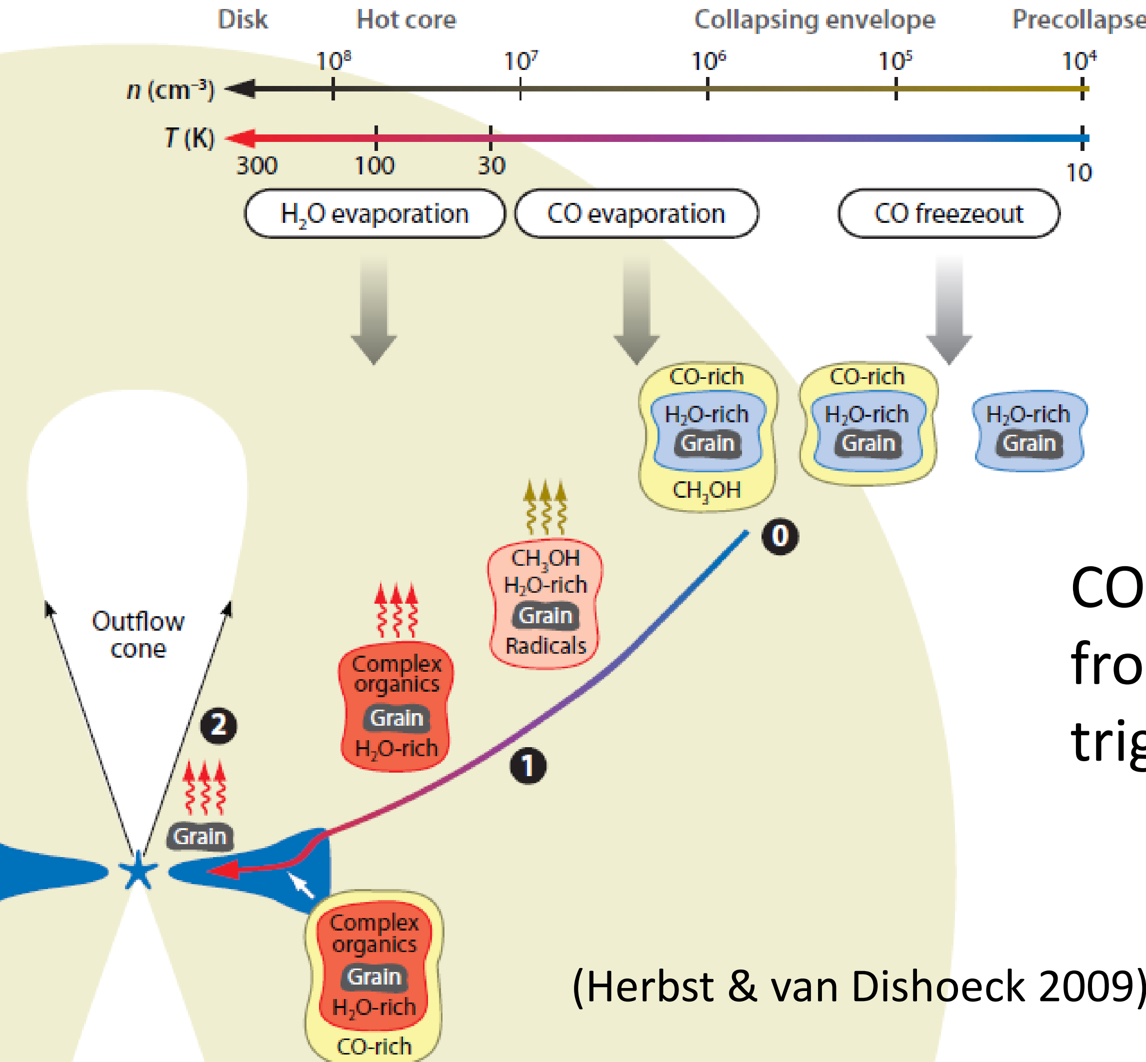
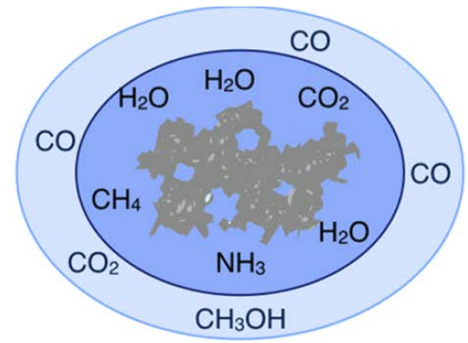
Chemical scenario: from simple molecules to complex molecules



(Herbst & van Dishoeck 2009)



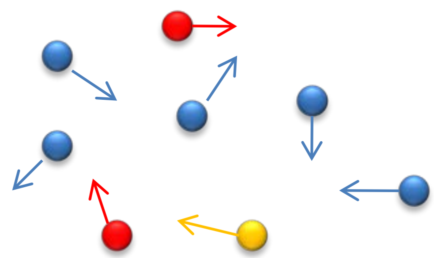
(Adapted from Oberg 2016)

COMs formation on icy grains from radical recombination triggered by phtotolysis

e.g., $CH_3O + CH_3 \rightarrow CH_3OCH_3$

Chemical processes in star-forming regions

Gas-phase



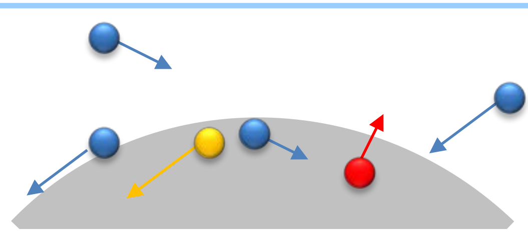
- イオンー分子反応を中心とした反応系
- 不飽和分子ができやすい

- Cosmic-ray ionization
- Ion-molecule reactions
- Neutral-Neutral reactions
- Photolysis etc...

cf. AB + C → A + BC

Adsorption **Desorption (thermal/non-thermal)**

Grain-surface



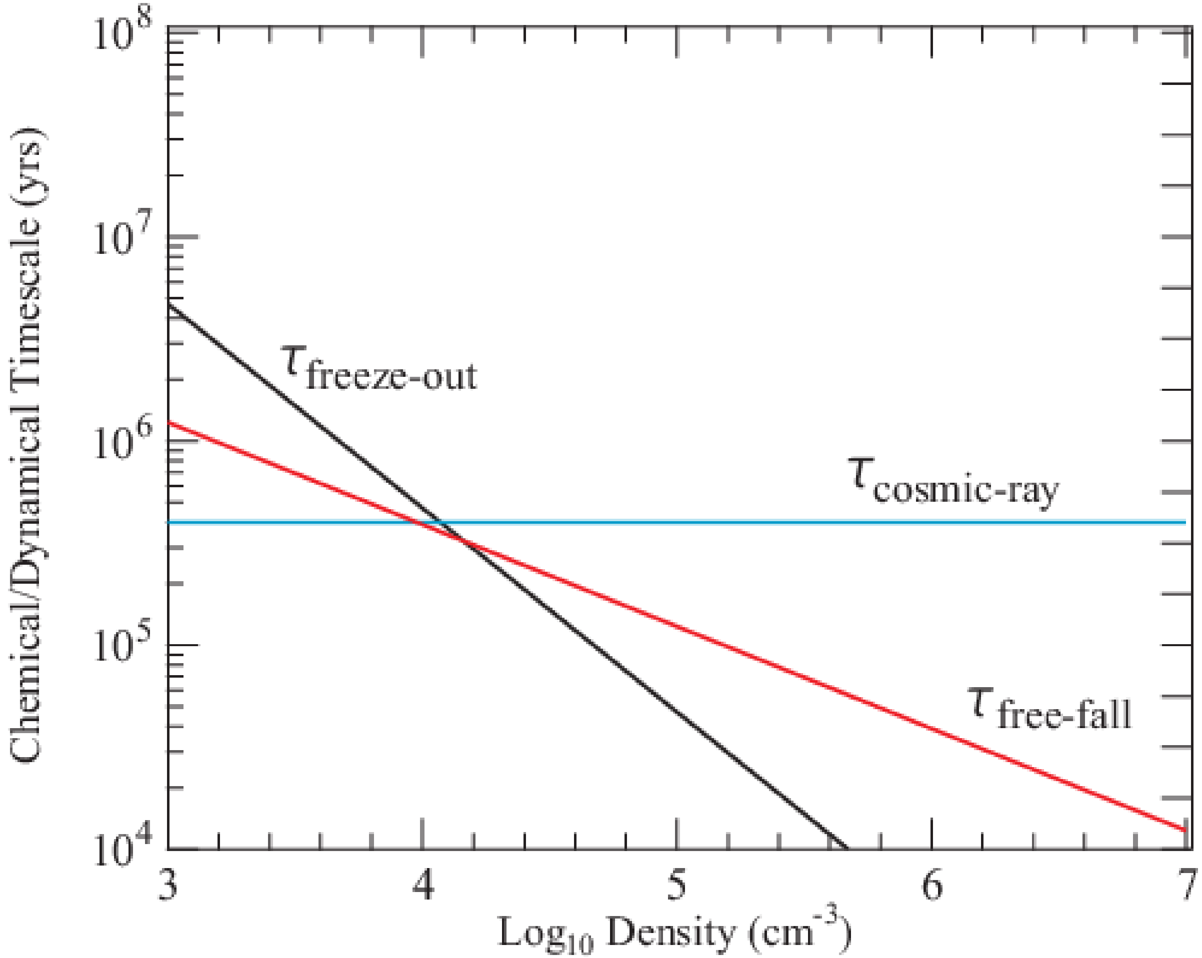
-飽和分子、大型分子ができやすい

- Hydrogenation: A +H → AH
- Reaction among heavy-element species

AB + C → ABC

Concentration of heavy-element species

Chemical and dynamical time scale



(based on Bergin & Tafalla 2007)

- **反応速度式:** $\displaystyle \frac{dn(i)}{dt} = \sum_j \boxed{\alpha_{ij}(T, F_{\mathrm{UV}})}\, n(j) + \sum_{j,k} \boxed{\beta_{ijk}(T, F_{\mathrm{UV}})}\, n(j)n(k)$

$$\beta = \boxed{AT^B} \exp\left(-\frac{\boxed{E_{\mathrm{act}}}}{T} \right)$$

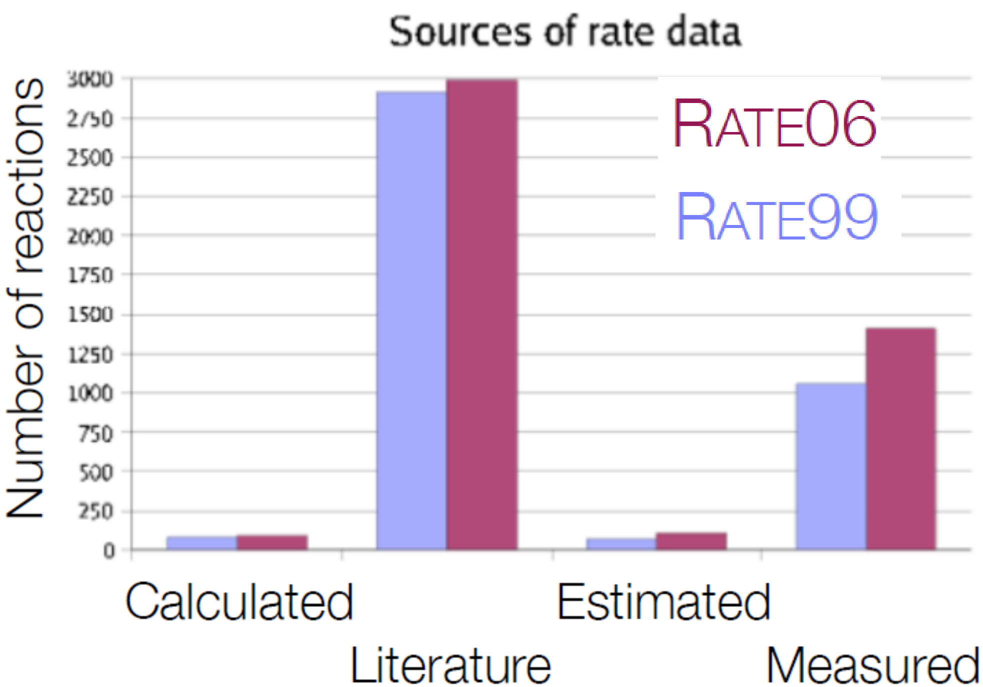
反応障壁

collision rate × 分岐比

- UMIST, kida 気相反応ネットワーク

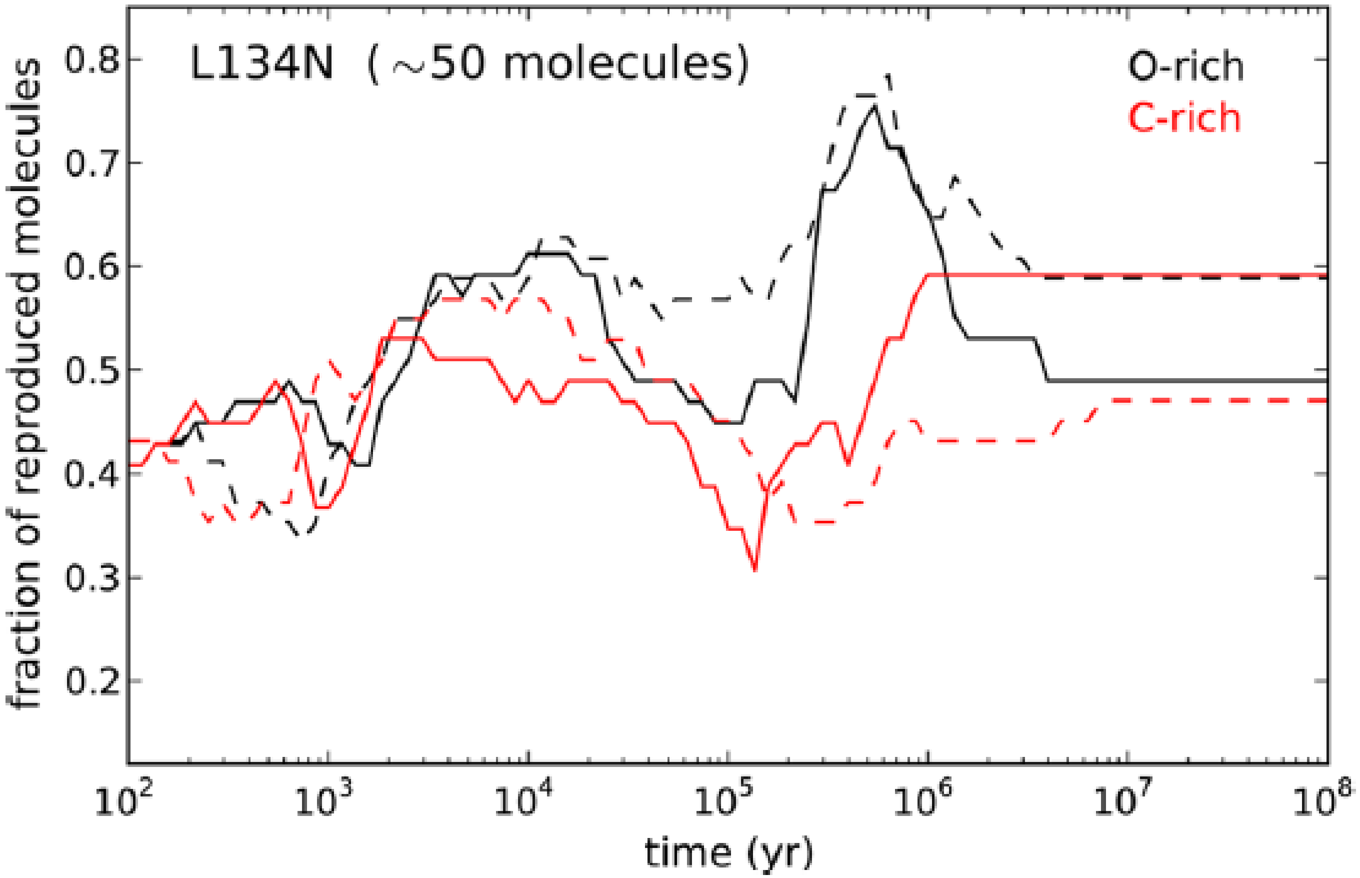
分子種 : ~500 (cf. ~160種が検出)
反応数 : ~5000

ABC + D → AB + CD
　　　　　 AD + BC



実験・計算に基づくものは1/3程度

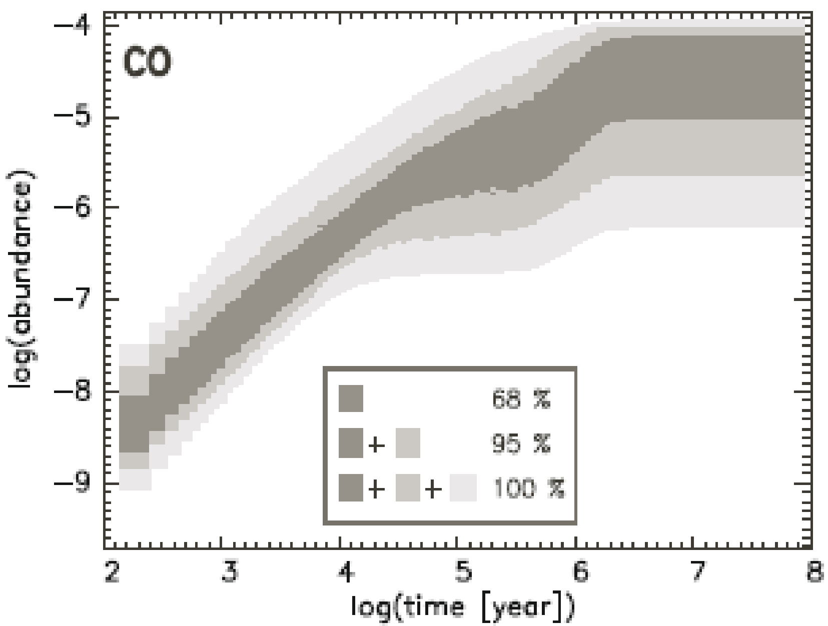
(Figure by C. Walsh)



(Agundez & Wakelam 2013)

不定性の解析(気相)

- 計算/実験データのない反応について反応速度係数を変えた計算
  ⇒ 系全体もしくは興味ある分子に影響を与える反応を抽出
  ⇒計算/実験



(Wakelam et al. 2010)

Table 1. Standard dense cloud model.

Parameter	Value
T	10 K
n_H	2×10^4 cm^{-3}
A_V	10
ζ_H	1.3×10^{-17} s^{-1}
Initial abundances	atomic except for 100% H_2
Rate coefficients	osu.03.2008

Table 2. Elemental abundances with respect to total hydrogen nuclei.

Table 3. Variational ranges of the parameters.

Parameter	Range	N runs
Reaction rate coefficients	Uncertainty Factor	2500
Temperature*	5–15 K	2500
H density*	$(1-3) \times 10^4$ cm^{-3}	—
Elemental abundances	±50%	2000
Cosmic-ray ionization rate (ζ)	$(0.5-5.0) \times 10^{-17}$ s^{-1}	1000
Initial Concentrations	see text	3500

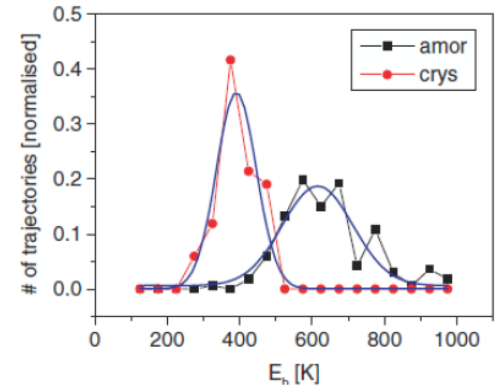
Notes. (*) Varied together.

ダスト表面化学の数値計算

- Rate equation method

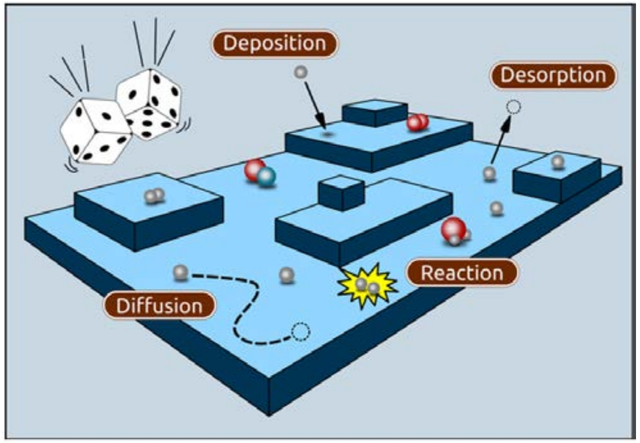
$$\frac{dn(i)}{dt} = \sum_j \alpha_{ij}(T, F_{\mathrm{UV}})n(j) + \sum_{j,k} \beta_{ijk}(T, F_{\mathrm{UV}})n(j)n(k)$$

  - Adv. : can be coupled with realistic dynamical models
  - Disadv. : not very accurate (e.g., back-diffusion, single binding energy)



(Al-halabi & van Dishoeck 2007)

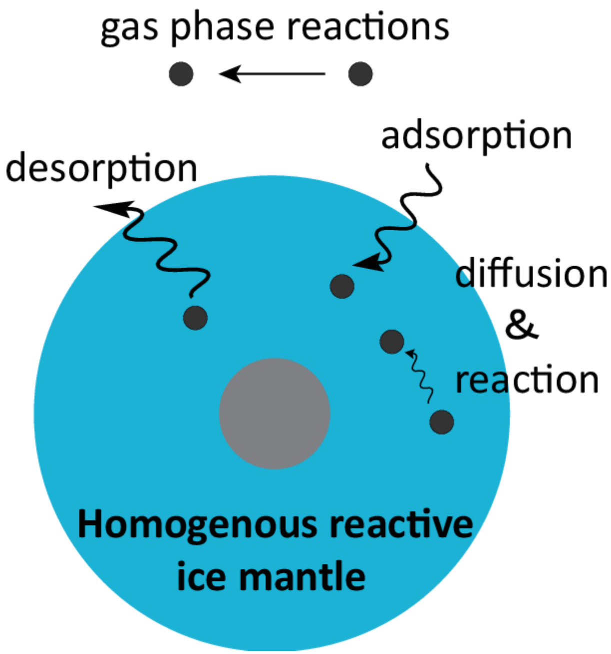
- Microscopic Monte Carlo method
  - Adv. : accurate
  - Disadv. : computationally expensive

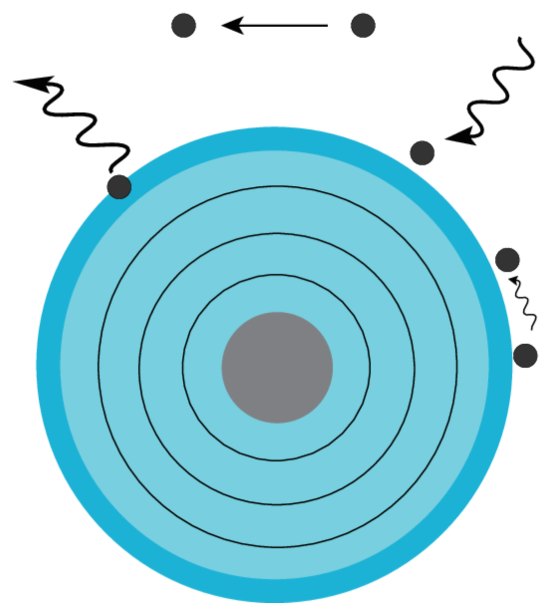


(Cuppen et al. 2013)

- 星間氷の主要構成分子については rate eq.でもfactor ~2以内で観測を再現可。COMs?

Modeling of gas-ice chemistry w/ rate eqs.

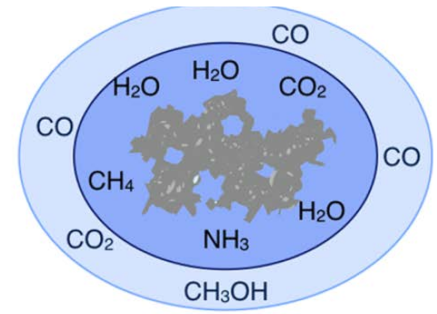




- 2 phase model
  (Hasegawa & Herbst 1992)
  - Gas
  - Homogenous reactive ice mantle

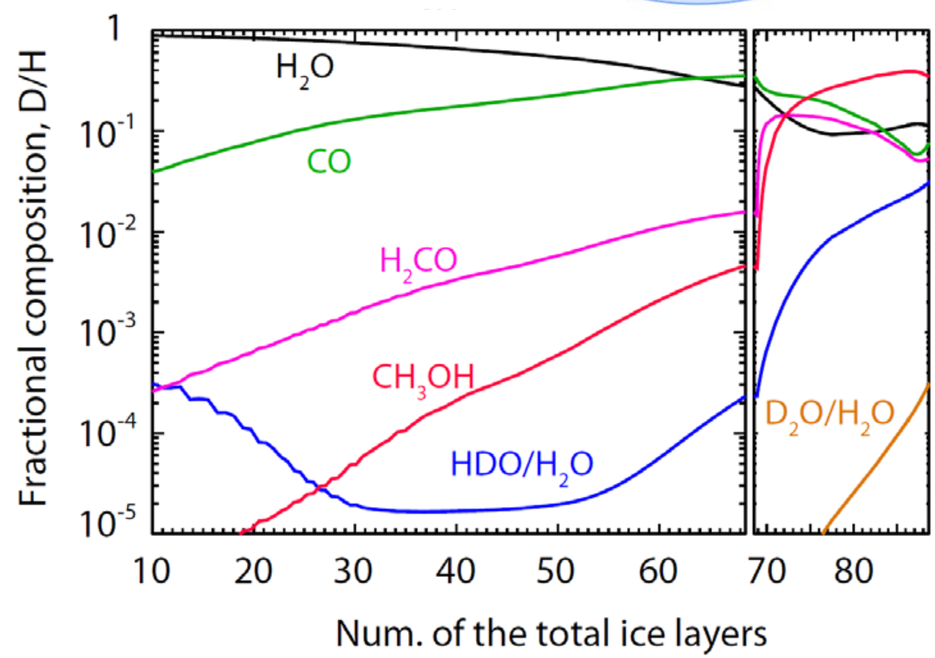
- (2+*n*)-phase model (Furuya et al. 2017)
  - Gas
  - Icy grain surface
  - Inhomogenous bulk ice mantle (distinct *n* phases)

非一様な氷マントル



- 氷マントルは非一様な構造を持つ

- バルク組成よりも層構造の理解が重要?



(Furuya et al. 2016)

- 最近の原始星コアの観測より (preliminary)
  D/H(COMs) ~ D/H(CH_3OH) ~ D/H(H_2CO) >> D/H(H_2O)

(Demyk+ 2010, Coutens+ 2016, Jorgensen+ 2016, 2017, Persson+ 2017)

まとめ

- 星形成領域の化学非平衡→反応速度式
- 反応係数、生成物の分岐比、etc.パラメータの決定がモデルの改善に重要
- 星間氷は層構造を持つ