Status of gas-grain astrochemical models

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Radiative-Magneto-Hydrodynamic simulations of star formation

Predictions

Observed abundances

Comparisons

Radiative transfer model

Predictions

Chemical model
Increasing complexity of chemical models

Chemistry
- Gas-phase chemistry
- Gas-phase chemistry + adsorption/desorption on grains
- Gas-phase chemistry + full surface treatment

Physics
- Fixed gas temperature, density and visual extinction
- Evolving gas temperature, density and visual extinction

Geometry
- 0D models
- 1D models (spherical)

Dynamic
- Static structure
- Infalling envelop

Increasing complexity of chemical models
Nautilus: gas-grain astrochemical model developed for the various ISM environments

Ruaud et al. in prep

Vidal et al. 2017 ++

Hincelin et al. 2016 ++

PDR : Le Gal et al. 2017

Wakelam et al. 2014 ++

Wakelam et al. 2016 ++
Chemical models

Solving the differential equations:

\[
\frac{dn_i(t)}{dt} = \sum_l \sum_j (k_{lj} n_l(t)n_j(t)) - n_i(t) \sum_j (k_{ij} n_j(t)) - k_{ads,i} n_i(t)n_{gr} + (k_{evap,i} + k_{crd,i}) n_i^s(t), \quad (2.1)
\]

\[
\frac{dn_i^s(t)}{dt} = \sum_l \sum_j (k_{lj} n_l^s(t)n_j^s(t)) - n_i^s(t) \sum_j (k_{ij} n_j^s(t)) + k_{ads,i} n_i(t)n_{gr} - (k_{evap,i} + k_{crd,i}) n_i^s(t), \quad (2.2)
\]

Parameters:
- Gas and dust temperature,
- Irradiation fields (UV, secondary UV, cosmic),
- Density of gas and dust,
- Initial conditions,
- Elemental abundances,
- Geometry of the source,
- Chemical network.
Nautilus: Gas-phase chemistry

Gas-phase reactions:
✓ Ion-molecule reactions ($A^+ + B \rightarrow C^+ + D$)
✓ Ionization and dissociation by cosmic-ray induced photons
✓ Electronic recombinations ($AB^+ + e^- \rightarrow A + B$)
✓ Neutral-neutral reactions ($A + B \rightarrow C + D$)
✓ Radiative associations ($A + B \rightarrow AB + \text{photon}$)
✓ Electron attachment ($C + e^- \rightarrow C^-$)

7506 gas-phase reactions and 489 species

Lots of works to improve the kinetic data:
- **Review of other key reactions** (*Wakelam et al. 2010*)
- **Importance of dielectric recombinations** (*Bryans et al. 2009*)
Nautilus: grain chemistry

« Rate-equations » based on Hasegawa & Herbst 1992 (+ evolutions):

→ Spherical grains: $r = 0.1 \mu m$

→ Homogeneous chemically active mantle
   Same properties through all the mantle for:
   • diffusion,
   • reactivity,
   • desorption

→ ~600 species coupled through ~6000 reactions

Slides from M. Ruaud
Nautilus: grain chemistry
Ruaud et al. (2016)

Mechanisms included in the code:

→ Diffusion:
  • Thermal
  • Tunneling effect

→ Reaction:
  • Langmuir-Hinshelwood
  • Eley-Rideal

→ Desorption:
  • Thermal
  • Chemical
  • Induced by cosmic-rays
  • Photodesorption

→ Dissociation:
  • Primary photons
  • Secondary photons

3-phase model

Slides from M. Ruaud
Formation des COMs à basse température : Compétition de réaction-diffusion

→ Pour les réactions ayant une barrière d’activation

\[ E_A < E_{\text{diff}}: \text{La réaction a plus de chance de prendre place que la diffusion de l’un des deux réactifs} \]
Formation des COMs à basse température : Résultats - diffusivité moyenne

Impact de la compétition de réaction diffusion

- Affecte la formation des molécules organiques complexes
  - HCO plus facilement produit: H+CO (E_A=2500K)
  - CH₃O aussi: H+H₂CO (E_A=2200K)

\[ \text{CH}_3\text{HCO} \rightarrow \text{CH}_3\text{CHO} \]
\[ \text{CH}_3\text{O} + \text{HCO} \rightarrow \text{HCOOCH}_3 \]

\[ \text{CH}_2\text{OH} \quad E_{\text{diff}}/E_{\text{des}}=0.4 \]

Sans compétition

Avec compétition

Ruaud et al. 2016

2-phase

Abondances en phase gaz

Transparent - thèse M. Ruaud
Comparison with gas-phase abundances in cold cores

- Comparison for about 60 species in the gas-phase (listed in Agundez & Wakelam 2013) and the full gas-grain chemical model Nautilus (Wakelam et al. 2015).

- The mean difference is better than a factor of 10 (approximately a factor of 6) at about $10^6$ yr.
## Comparison with ice abundances

<table>
<thead>
<tr>
<th>Modèle</th>
<th>time [yr]</th>
<th>H$_2$O</th>
<th>CO</th>
<th>CO$_2$</th>
<th>CH$_3$OH</th>
<th>NH$_3$</th>
<th>CH$_4$</th>
<th>H$_2$CO</th>
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<tbody>
<tr>
<td>2-phase model</td>
<td>2.0x10$^6$</td>
<td>100</td>
<td>55</td>
<td>0.05</td>
<td></td>
<td>5</td>
<td>30</td>
<td>18</td>
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<tr>
<td>3-phase model</td>
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<td>23</td>
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<td>6</td>
<td>2</td>
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<tr>
<td>Low mass YSOs</td>
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<td>100</td>
<td>12-35</td>
<td>23-37</td>
<td>5-12</td>
<td>4-8</td>
<td>3-6</td>
<td>~6</td>
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<tr>
<td>Massive YSOs</td>
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<td>100</td>
<td>4-14</td>
<td>12-25</td>
<td>5-23</td>
<td>~7</td>
<td>1-3</td>
<td>~2-7</td>
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<td>Toward BG stars</td>
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<td>20-43</td>
<td>18-39</td>
<td>6-10</td>
<td>&lt;7</td>
<td>&lt;3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Ruaud et al. (2016)
Predictions on ice composition in cold cores

HCN, N₂, CH₃CHO, HCOOH, HCO, CH₃O,...
Chemistry during cold core formation

Extracting the time-dependent physical parameters of cells of material forming several cold cores

Bonnell et al., 2013
Histories used as input parameters of the chemical model.

Species abundances computed during the formation of cold cores

Ruaud et al. in prep
Column density maps for two different clouds

Cloud A

Cloud B

Ruaud et al. in prep

Black contours were added for clarity and indicates log(NH) from 21 to 23.
Carbon chains in two different clouds

- Much larger column densities of carbon chains in cloud B with respect to cloud A.

- Difference in electronic fraction and C/O elemental ratio. -> difference in history of the material.
Intermediate density pre-phase in cloud B reduces the electronic fraction of the cloud and increases the C/O ratio due to the formation of water at the surface of grains.
Binding energies: keys for diffusion (for the moment) and desorption

Simple method to estimate the binding energies ($E_D$) for missing data (mostly radicals) + other updates from the literature (Wakelam et al. 2017).

79 modified values (important in some cases).

- **CH$_3$** (1175K C+$(3/4)$(CH$_4$-C) -> 1600K Wakelam et al.),
- **HCO** (1600K CO+H -> 2400K Wakelam et al.)
New \( E_D \) + diffusion of by tunneling effect O (Minissale et al. 2013)
Binding energies: keys for diffusion (for the moment) and desorption

Impact of the model of chemical desorption

Fig. 2 Gas phase abundances of CH$_3$OH (solid lines), CH$_3$CNH$_2$ (dashed lines), and CO$_2$ (dotted lines) computed with the RRK (black lines) or the MDCH (grey lines) formalisms as a function of time.

Model from Garrod et al. (2017)
Model from Minissale et al. (2016)
3DICE group
(Bordeaux astrochemical group)

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Funding

KInetic Database for Astrochemistry
http://kida.obs.u-bordeaux1.fr/

AstroChemical Newsletter
http://acn.obs.u-bordeaux1.fr/

InterStellar Abundance database
http://isa.obs.u-bordeaux1.fr/

Nautilus gas-grain code
(upon request)

KIDA 2017 26 au 29 septembre
Bordeaux (France)
Impact du modèle de désorption chimique


Probabilité de désorption : \[ P = \left(1 - \frac{E_D}{E_{\text{reac}}} \right)^{s-1} \]

Fraction de molécules qui désorbe : \[ f = \frac{aP}{1 + aP} \]

\( a \) est le nombre de modes vibratoires dans la molécule/surface-bound system.

\( a = \frac{\nu}{\nu_S} \), and \( \nu \) is the surface-molecule bond-frequency and \( \nu_S \) the frequency at which the energy is lost to the grain surface.

a n’est pas connu et généralement pris entre 0.01 and 0.1, identique pour toutes les espèces.
Binding energies : clés pour la diffusion et la désorption

Impact du modèle de désorption chimique

Modèle Minissale et al. (2016) - basé sur des résultats expérimentaux de réactions de surface O+H, CO+H, O+O et N+N

Fraction de molécule qui désorbe :

\[ f = e^{-\frac{E_D}{\epsilon E_{\text{reac}}/N}} \]

N the number of degree of freedom’s of the produced molecule \((N = 3n)\) and \(\epsilon\) is the fraction of the energy kept by the product with a mass \(m\)

Résultats expérimentaux sur de la glace d’eau montrent une désorption beaucoup moins efficace que sur des surfaces nues. Pour la plus part des systèmes, la détection est en dessous du seuil de détection. \(\epsilon\) inconnu pour des surfaces d’eau.

Recommandation des auteurs : Calcul de \(f\) pour des surfaces nues puis divisé par 10. Utiliser les valeurs mesurées pour les systèmes \(f_{O+H} = 30\%\), \(f_{OH+H} = 25\%\) and \(f_{N+N} = 50\%\)