PDR Modelling with KOSMA-\(\tau\)

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The KOSMA-τ PDR Code

- 1-D, spherical geometry
  - power-law density profile
  - isotropic illumination
- self-consistent solution of energy- and chemical balance and radiative transfer
- full dust RT and temp. computation for varying dust distribution
The KOSMA-τ PDR Code

- 1-D, spherical geometry
  - power-law density profile
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- self-consistent solution of energy- and chemical balance and radiative transfer
- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
  - stochastic clump ensemble
Chemistry in KOSMA-\(\tau\)

- Rate equation approach
- Steady-state chemistry
  - LAPACK: DGESV, DGELSD (least squares), DGESVX (w. equilibration)
- Modular chemistry
  - User selects species, code selects reactions, creates conservation equations and computes Jacobian
- Isotopologue chemistry: \(^{13}\text{C}\) and \(^{18}\text{O}\)
  - Update to the fractionation reaction from Langer et al. 84 (Mladenovic & Roueff, 2014)
  - Isotopic reaction set (Röllig et al. 2013)
- Standard database: UDfA 2012 (McElroy et al. 2013)
Chemistry in KOSMA-τ

- Standard database: UDfA 2012
  - reactions with $H_2^*$ overcome activation energy
  - $CH^+$ and $SH^+$ formation (Agundez et al. 2010, Nagy et al. 2012)
  - cyclic and linear-isomers included (new branching ratios from Chabot et al. 2013) with all isotopologues
    - $l$-C$_3$H$_3^+$, $l$-C$_3$H$_2^+$, $l$-C$_3$H$_2$, $l$-C$_3$H
  - additions
    - Fluorine chemistry (Neufeld et al. 2005)
    - Photodissociation of CS$_2$, N$_2$O
      (van Dishoeck et al.)
  - $H_2$ formation
    - Chemi- & physisorption
      (Cazaux & Tielens 2002,04,10)
Full Surface Chemistry Upgrade

- Coupling of gas-phase and surface chemistry
- Steady-state chemistry
- Rate equation approach (Hasegawa et al. 1992, 1993)
- Processes included:
  - adsorption
  - desorption only from 2 top layers (Aikawa et al. 1996)
    - thermal desorption (binding energies from UDfA + updates)
    - photo-desorption (photo cross-section like gas-phase)
      photo-dissociative desorption (eg. JH₂O +hv → OH + H  Andersson+ 08)
    - photo-dissociation on grains (equivalent to gas-phase)
    - CR induced photo-desorption/diss. (Hasegawa & Herbst 1993)
    - H₂-formation induced desorption (Willacy et al. 1994, 2007)
    - chemistry induced desorption (Minissale et al. 2015, Cazaux et al. 2015)
  - surface-surface processes (Langmuir-Hinshelwood)
\( n = 10^4 \text{ cm}^{-3} \)
\( \chi = 10^4 \)

small chemical network
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Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption (Minissale et al. 2015, Cazaux et al. 2016)
Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of the product (Minissale et al. 2015, Cazaux et al. 2016)

\[
P_{des} = e^{-\frac{E_{bind}}{\epsilon \Delta H_r / N}}
\]

\[
E, p \text{ conservation} \\
\epsilon = \frac{(M - m)^2}{(M - m)^2}
\]
Chemical details with impact

Esplugues et al. 2016

KOSMA-τ with „comparable“ setup
Chemical details with impact

$\rightarrow$ significantly different ice composition

Esplugues et al. 2016

KOSMA-$\tau$ with “comparable” setup

plus

(theoretical BRs)

$\text{JCO} + \text{JO} \rightarrow \text{CO}_2$ (22%)

$\text{JCO} + \text{JO} \rightarrow \text{JCO}_2$ (78%)
Chemical details with impact

Esplugues et al. 2016

→ significantly different ice composition

KOSMA-τ with „comparable“ setup

plus

(measured BRs)

JCO + JO → CO₂  (4%)

JCO + JO → JCO₂  (96%)

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Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of both products (Minissale et al. 2015, Cazaux et al. 2016)

\[
P_{\text{des}} = e^{-\frac{E_{\text{bind}}}{\epsilon \Delta H_r / N}}
\]

\[
1 - P_{\text{des}}
\]

\[
E, p \text{ conservation}
\]

\[
\epsilon = \frac{(M - m)^2}{(M - m)^2}
\]
Full Surface Chemistry Upgrade

- So far assumed that all products desorb with full reaction enthalpy
- Now, we assume that formation energy is distributed across products
  - analogue to free particle decay: \[ \frac{E_1}{E_2} = \frac{m_1}{m_2}, \quad \frac{E_1}{E_{\text{tot}}} = \eta_1 = \frac{m_1}{m_1 + m_2} \]
  - \( P_{\text{des}, i} = e^{-\frac{E_{\text{bind}, i}}{\epsilon \eta_1 \Delta H_i / N_i}}, \quad P_{\text{des}, i} = 1 - P_{\text{des}, i} \)
  - \( \text{H}_2 \) always desorbs

\[
(1 - P_{\text{des}, 1}) \times (1 - P_{\text{des}, 2}) \quad (1 - P_{\text{des}, 1}) \times P_{\text{des}, 2} \quad P_{\text{des}, 1} \times (1 - P_{\text{des}, 2}) \quad P_{\text{des}, 1} \times P_{\text{des}, 2}
\]

Röllig et al., in prep
Some example branching rates

- $\text{JOH} + \text{JO} \rightarrow$
  - $\text{O}_2 + \text{H} \quad 7 \times 10^{-5} (0.019)$
  - $\text{JO}_2 + \text{H} \quad 5.7 \times 10^{-4} (-)$
  - $\text{O}_2 + \text{JH} \quad 0.11 (-)$
  - $\text{JO}_2 + \text{JH} \quad 0.89 (0.981)$

- $\text{JH}_2\text{O}_2 + \text{JH} \rightarrow$
  - $\text{H}_2\text{O} + \text{OH} \quad 0.002 (0.021)$
  - $\text{JH}_2\text{O} + \text{OH} \quad 0.16 (-)$
  - $\text{H}_2\text{O} + \text{JOH} \quad 0.01 (-)$
  - $\text{JH}_2\text{O} + \text{JOH} \quad 0.83 (0.979)$

- $\text{JHCO} + \text{JH} \rightarrow$
  - $\text{CO} + \text{H}_2 \quad 0.65 (0.47)$
  - $\text{JCO} + \text{H}_2 \quad 0.35 (-)$
  - $\text{CO} + \text{JH}_2 \quad 0 (-)$
  - $\text{JCO} + \text{JH}_2 \quad 0 (0.53)$

BRs depend on the energy redistribution.
Other distribution schemes?
Questions & Concerns

- Binding energies – Yes, but which one? (see Wakelam et al. 2017)
- How about surfaces of very small grains? PAHs?
  - Very important for H₂ formation
  - Excitation of small hydrocarbons, H₂, high-J CO
- Cross sections of surface photo-processes
  - Important for PDRs because of FUV attenuation/shielding
  - Photodesorption yields?
- Numerical stability? Convergence/steady-state?
  - Including/excluding of
    - Desorption processes
    - Grain + gas phase species
    - Initial abundances! PDRs are different from dark cloud models
  - Any technical/numerical comments in your papers are much appreciated.
- (Column) density is no observable.
Density is no observable
Column density is no observable

![Graphs showing the relationship between $A_V$ and column density for different species in gas and gas-dust phases.](image)
Line intensities are observed

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<th>∫ T_{mb} dv [K km/s]</th>
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<td>CO J=3-2</td>
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<td>CO J=4-3</td>
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<td>[CII] 158µm</td>
<td>2.3</td>
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<td>[CI] 609 µm</td>
<td>8.7</td>
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<tr>
<td>[CI] 370µm</td>
<td>2.3</td>
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</tbody>
</table>

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<tbody>
<tr>
<td>CO J=1-0</td>
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<tr>
<td>CO J=2-1</td>
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<td>CO J=4-3</td>
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<td>[CII] 158µm</td>
<td>2.1</td>
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<td>2.6</td>
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</table>

lower column densities
higher intensities!
Excitation matters

gas cooling is significantly reduced in the absence of CO

→ gas temperature increases
Questions & Concerns

• Densities and column densities are good for inter-model comparison but are no observables.
• Calibrate model against 'derived' (column) densities? Which ones? Derived under which conditions?
  – We need to make sure that model (column) densities can be compared to 'observed' ones.
• Alternatively one could apply radiative transfer and compare against measured intensities!
  – But then we need to know the density/temperature structure.

It might be time for a follow-up round of the PDR-Benchmark.
Thank you for your attention!