Data Needs for Astrochemical Models

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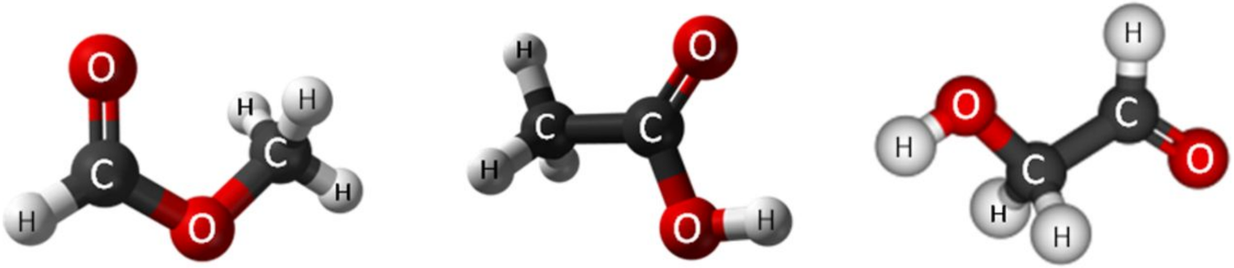

Methyl formate   Acetic acid   Glycolaldehyde

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Formation of Molecules

Wide temperature range
~ 5 – 4000 K

Wide density range
n ~ 50 – 10^{14} cm-3

Wide radiative flux range
G ~ 0 – 10^5 G_{ISM}

Wide range of chemical processes
One-body, two-body and three-body gas phase processes
Surface reactions on ices
Bulk reactions on ices
Gas-solid interaction

Sometimes difficult to study relevant processes in the laboratory or theoretically

Wide range of applications – the early universe to star formation to late stages of stellar evolution (AGB stars, PNe, Sne) to exoplanet

One-body reactions

Photodissociation/photoionisation:

$$\boldsymbol{\beta = \beta_0 \exp(-bA_V)}$$

where **b** is a constant (~ 1- 3) and differs for different molecules, $\boldsymbol{\beta_0}$ is the unshielded rate in the ISM.

Details depend on wavelength dependence of photo cross-sections, wavelength dependence of the incident UV flux and dust grain properties.

Cosmic-ray ionisation of H_2 and He

Details sensitive to (low energy) CR energy spectrum and flux

Two-body reactions

Ion-neutral reactions

Neutral-neutral reactions

Ion-electron dissociative recombination

(molecular ions)

Ion-electron radiative recombination

(atomic ions)

Mutual Neutralisation (cation-anion)

Radiative association

Three-body reactions (only if density is very large, $> 10^{12}$ cm^{-3})

Molecular Emission in PPDs

- A good physical model – stellar properties, mass accretion rate, dust properties, stellar and interstellar UV, stellar Lyman alpha radiation, CR, X-ray fluxes, geometry, irradiation from a nearby O-type star
- A good chemical model – reaction rates including high T and 3 body rates, gas-grain interchange, surface chemistry, .. (UMIST Database for Astrochemistry www.udfa.net)
- A good radiative transfer model – UV photons (input radiation), IR and (sub)millimeter photons (output radiation), collisional & radiative rate coefficients,..

Chemistry in PPDs

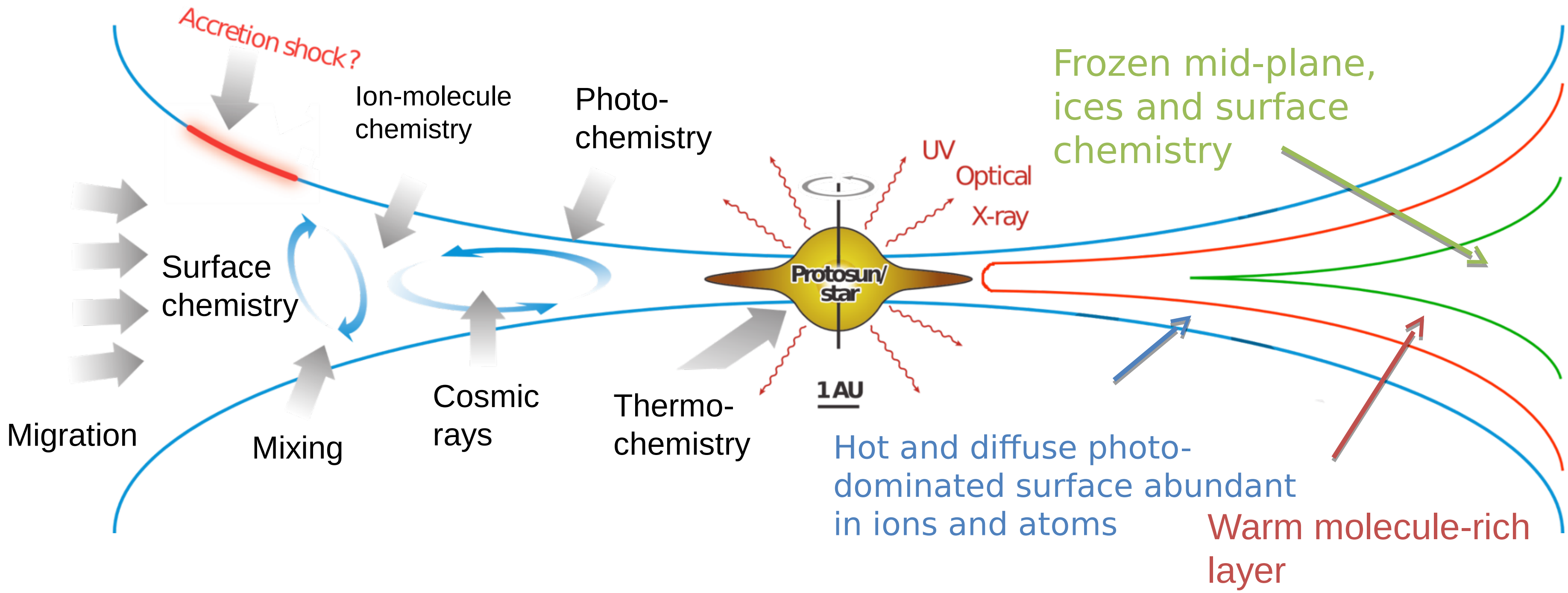
Walsh, Millar & Nomura 2010, ApJ, 722, 1607

Heinzeller, Nomura, Walsh & Millar, 2011, ApJ, 731, 115

Walsh, Nomura, Millar & Aikawa 2012, ApJ, 747, 114

Large gradients in physical parameters give rise to small scale abundance and (sometimes large) emission variations

Protoplanetary Disks



Extent of each layer depends on physical conditions

Fig. from Mumma & Charnley, 2011, ARAA, 49, 471

Surface Chemistry

Network from Garrod & Herbst, 2006;

Garrod et al. 2008; Laas et al. 2011

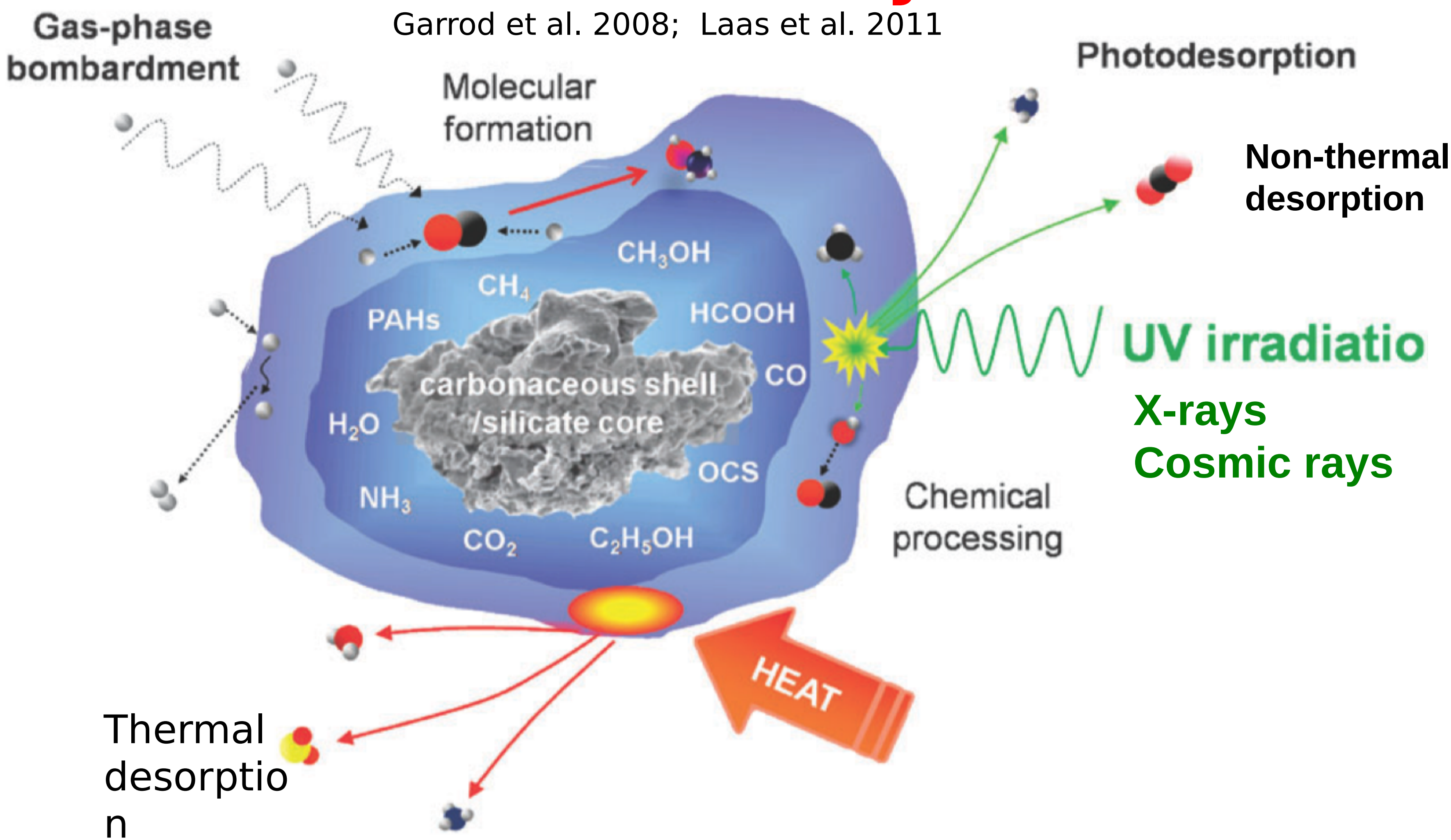
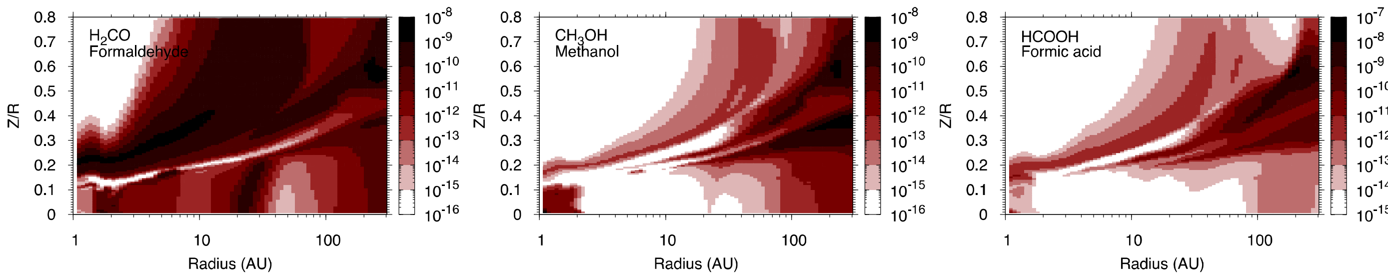
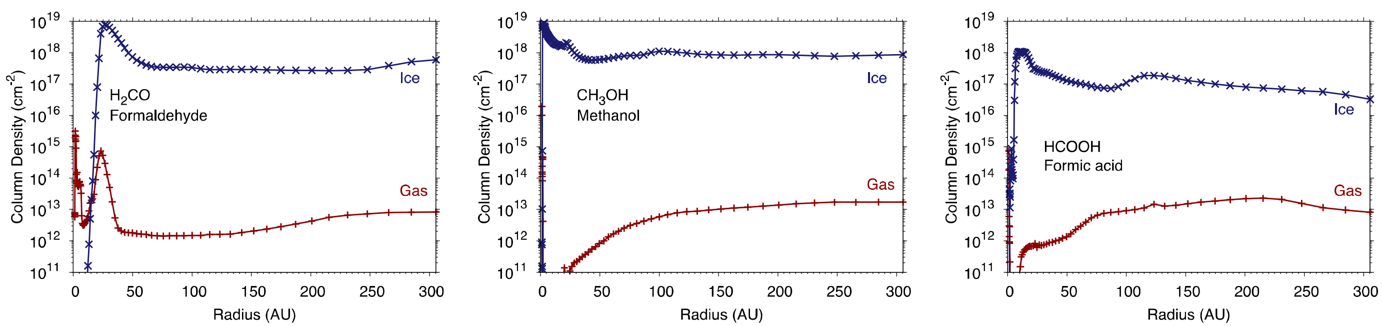


Figure from Burke & Brown 2010, PCCP, 12, 5947

Molecular Distributions

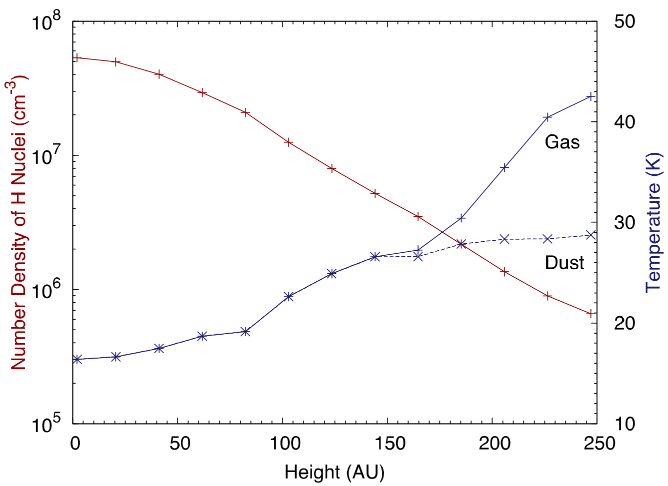


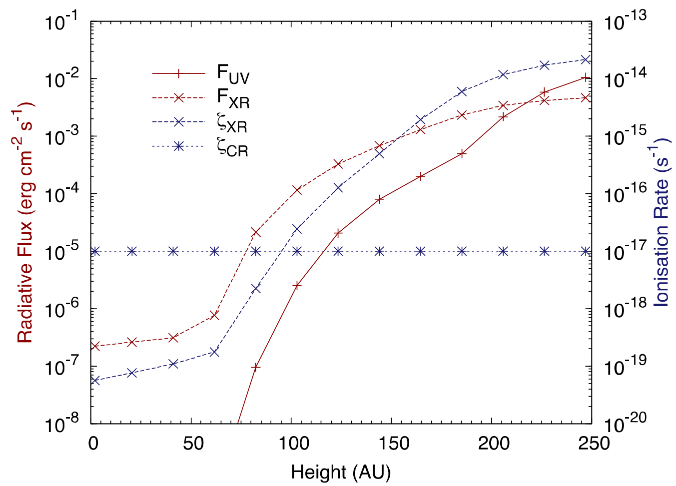
Model 5 – fractional abundances over disk



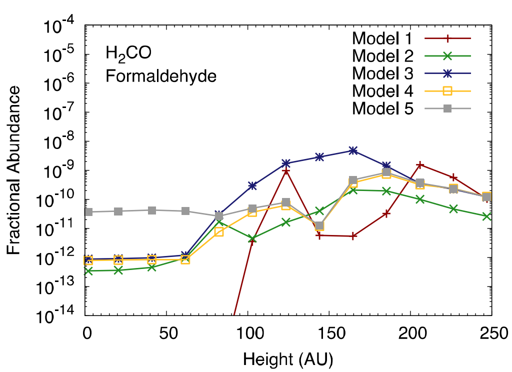
Vertical column densities of gas-phase and solid-state species. Individual species have their own ‘snow-lines’ depending on their binding energy

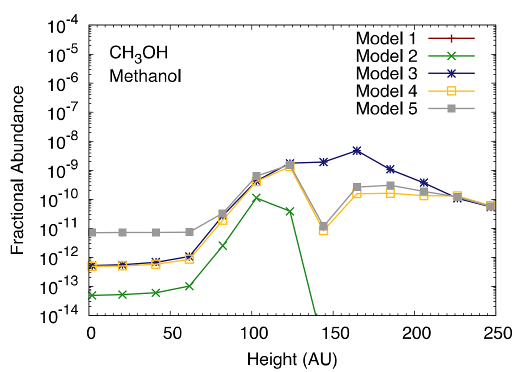
COMs Models - Vertical Profiles at 305 AU

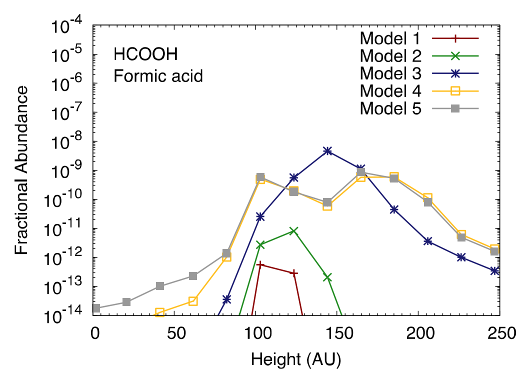




Radius = 305 AU – Gas warmer than dust at disk surface (LHS)
Cosmic rays dominate ionisation below 90 AU, X-rays have largest radiative flux below 150AU (RHS)

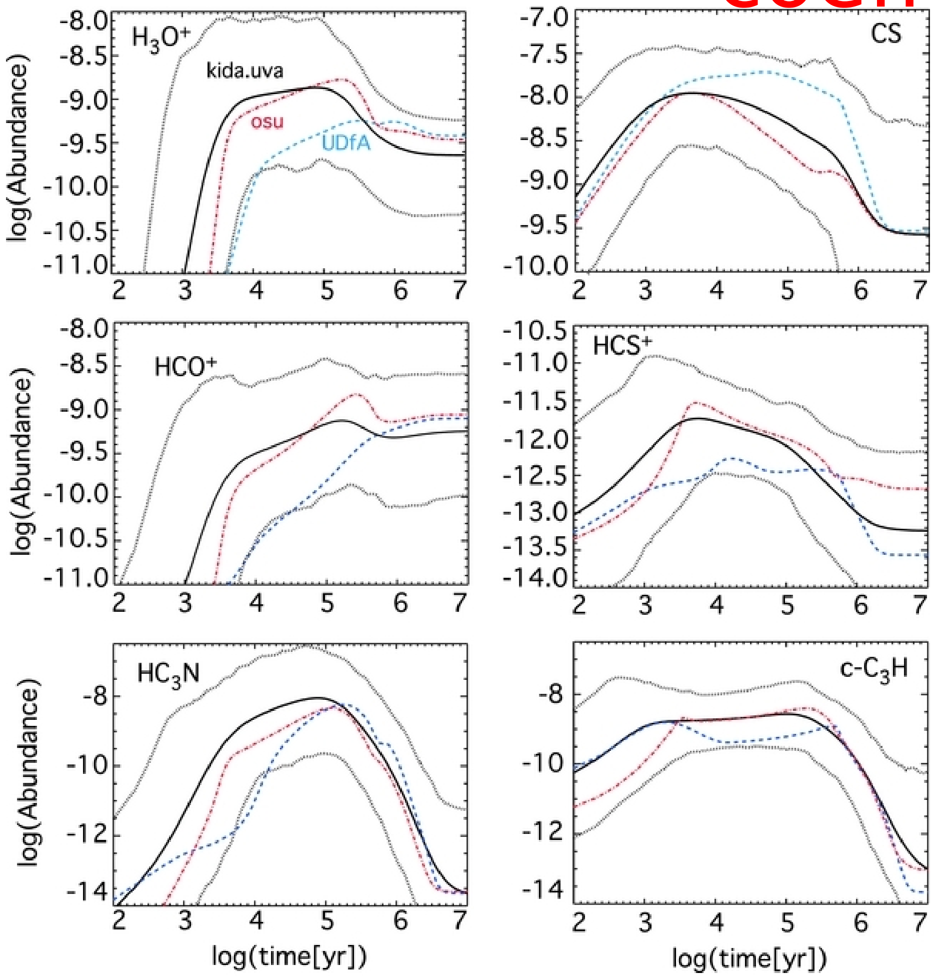






Model 1: thermal desorption, Model 2: non-thermal desorption, Model 3: surface chemistry, Model 4: Radiation processing, Model 5: Reactive

The effect of uncertainty in rate coefficients



- Between databases (KIDA, OSU, UDFA)
- Intrinsic within databases. Dotted lines show 2-sigma uncertainties in abundances
- Important to identify key reactions for further study

KInetic Database for Astrochemistry (KIDA)
Wakelam et al. 2012 ApJS 199 21

Discussion Points

How do we advance the subject?

Gas-phase kinetics

Ion-neutral – well studied in lab, well described theoretically

Neutral-neutral – well studied in lab (but not at low T), well described theoretically, with some surprises and some difficulties

Recombination – of complex ions with electrons and anions

Role of top-down chemistry, e.g. driven by destruction of PAHs

Photodissociation/photoionisation

Grain surface processes

Binding energies, mobilities, reaction vs. diffusion – some aspects well studied in lab, but many important exceptions

Reaction processes and rates – few systems studied

Non-thermal desorption – few systems studied (mostly photo-desorption)

Issues

No agreed definition of 'IS' or water ice

Exponential dependence of surface processes on T_d