Rate Kinetics Models

- Given local ρ, T, A_v, etc. - evolves initially atomic* gas through time using reaction network
- 12 elements; $\approx$ 1200 chemical species; $\approx$ 12000 reactions
- Three phase model - gas, grain surface, and ice mantle
- Static or collapsing cloud
- Included reactions: CR ionization, photoionization, ion-molecule, charge transfer, neutral exchange, dissociative recombination, radiative association, radiative recombination, grain surface reaction, photodesorption

1
00:00:10,870 --> 00:00:09,270
so as you said i'm tyler this work was

2
00:00:12,310 --> 00:00:10,880
done with my advisor rob garrett at

3
00:00:15,430 --> 00:00:12,320
cornell

4
00:00:17,189 --> 00:00:15,440
this is going to be again modeling so

5
00:00:19,590 --> 00:00:17,199
not as many pretty pictures

6
00:00:20,710 --> 00:00:19,600
but some plots

7
00:00:22,390 --> 00:00:20,720
the work is

8
00:00:24,470 --> 00:00:22,400
going to be looking at the effects that

9
00:00:25,590 --> 00:00:24,480
a grain size distribution would cause to

10
00:00:27,189 --> 00:00:25,600
a model

11
00:00:29,349 --> 00:00:27,199
i'm going to explain a lot i have plenty

12
00:00:30,950 --> 00:00:29,359
of warm-up slides as well so plenty of

13
00:00:32,790 --> 00:00:30,960

background to get through first

14
00:00:34,229 --> 00:00:32,800
so let's just get on to that um the

15
00:00:36,069 --> 00:00:34,239
major background questions that this

16
00:00:37,750 --> 00:00:36,079
work is going to try and address

17
00:00:39,990 --> 00:00:37,760
is where and how could chemical

18
00:00:41,590 --> 00:00:40,000
complexity thrive and again coming from

19
00:00:42,869 --> 00:00:41,600
an astronomy department we're not

20
00:00:44,950 --> 00:00:42,879
talking about

21
00:00:46,630 --> 00:00:44,960
things like you know rocks

22
00:00:48,709 --> 00:00:46,640
or atmospheres even

23
00:00:50,389 --> 00:00:48,719
but molecular clouds so these molecular

24
00:00:51,910 --> 00:00:50,399
clouds or interstellar clouds are the

25
00:00:53,189 --> 00:00:51,920
places where stars are forming and

26
00:00:55,430 --> 00:00:53,199
eventually planets will form around

27
00:00:57,029 --> 00:00:55,440
those stars

28
00:00:58,150 --> 00:00:57,039
so to look at those regions you want to

29
00:00:59,670 --> 00:00:58,160
think about what environmental

30
00:01:02,389 --> 00:00:59,680
parameters you need to think about

31
00:01:04,070 --> 00:01:02,399
densities temperatures uv field

32
00:01:05,990 --> 00:01:04,080
strengths

33
00:01:07,670 --> 00:01:06,000
you need to look at chemical pathways

34
00:01:10,149 --> 00:01:07,680
this is where the laboratory chemists

35
00:01:12,149 --> 00:01:10,159
come in they need to tell us what

36
00:01:13,429 --> 00:01:12,159
reactions we should be thinking about

37
00:01:15,030 --> 00:01:13,439
what barriers they have what rate

38
00:01:15,830 --> 00:01:15,040

constants we need to put into our models

39
00:01:16,710 --> 00:01:15,840
for

40
00:01:17,670 --> 00:01:16,720
um

41
00:01:19,350 --> 00:01:17,680
we're i'm going to be looking at the

42
00:01:20,550 --> 00:01:19,360
building blocks for complex species so

43
00:01:22,390 --> 00:01:20,560
this is kind of breaking it down to the

44
00:01:24,070 --> 00:01:22,400
very beginning like brett showed in the

45
00:01:26,789 --> 00:01:24,080
warm-up talk this will be looking at

46
00:01:29,030 --> 00:01:26,799
things closer to methane and water and

47
00:01:31,429 --> 00:01:29,040
methanol rather than methyl formator

48
00:01:32,550 --> 00:01:31,439
anything more complex than that

49
00:01:33,910 --> 00:01:32,560
and then the model parameters that i

50
00:01:35,830 --> 00:01:33,920
need to put into my model to make this

51
00:01:37,910 --> 00:01:35,840
thing work so again plenty of rate

52
00:01:39,670 --> 00:01:37,920
constants plenty of barriers and plenty

53
00:01:40,390 --> 00:01:39,680
of chemical species

54
00:01:42,789 --> 00:01:40,400
so

55
00:01:44,950 --> 00:01:42,799
applying this model to a quiescent dark

56
00:01:46,630 --> 00:01:44,960
cloud

57
00:01:49,030 --> 00:01:46,640
quiescent just means it's static it's

58
00:01:51,030 --> 00:01:49,040
not yet collapsing it's not entering the

59
00:01:52,469 --> 00:01:51,040
protostellar phase so it's it's fairly

60
00:01:53,590 --> 00:01:52,479
boring as you might

61
00:01:55,350 --> 00:01:53,600
want to say

62
00:01:58,389 --> 00:01:55,360
but it is a large region region of over

63
00:01:59,590 --> 00:01:58,399

density um the density here is around 10

64
00:02:01,749 --> 00:01:59,600
to the four particles per cubic

65
00:02:03,190 --> 00:02:01,759
centimeter um

66
00:02:05,350 --> 00:02:03,200
i think most people could realize that's

67
00:02:06,630 --> 00:02:05,360
a fairly low number it's a pretty good

68
00:02:08,070 --> 00:02:06,640
vacuum

69
00:02:10,710 --> 00:02:08,080
but it's still more dense than your

70
00:02:12,710 --> 00:02:10,720
average interstellar space um an average

71
00:02:15,110 --> 00:02:12,720
dark cloud uh interstellar cloud has a

72
00:02:17,910 --> 00:02:15,120
total mass of uh 10 000 to a million

73
00:02:19,589 --> 00:02:17,920
solar masses solar mass again

74
00:02:21,830 --> 00:02:19,599
you know the mass of the sun 10 to the

75
00:02:22,949 --> 00:02:21,840
30 kilograms so it's a lot of a lot of

76
00:02:24,790 --> 00:02:22,959
mass

77
00:02:26,630 --> 00:02:24,800
and the places i'm looking at uh have a

78
00:02:28,390 --> 00:02:26,640
temperature of around 10 kelvin so the

79
00:02:31,270 --> 00:02:28,400
low end of these spectra that have been

80
00:02:32,390 --> 00:02:31,280
shown in the terahertz

81
00:02:34,550 --> 00:02:32,400
we're going to assume some elemental

82
00:02:36,869 --> 00:02:34,560
abundances for this model with respect

83
00:02:39,910 --> 00:02:36,879
to total hydrogen um showing that i have

84
00:02:41,350 --> 00:02:39,920
a pseto ratio of about 0.5 that can vary

85
00:02:42,470 --> 00:02:41,360
it depends on what stars you're around

86
00:02:43,910 --> 00:02:42,480
or what stars are affecting the

87
00:02:45,830 --> 00:02:43,920
environment

88
00:02:47,430 --> 00:02:45,840

but this is just what i've used

89
00:02:48,550 --> 00:02:47,440
and the model will involve more elements

90
00:02:49,990 --> 00:02:48,560
but these are the only ones that really

91
00:02:51,589 --> 00:02:50,000
matter

92
00:02:52,550 --> 00:02:51,599
you can see that i list atomic hydrogen

93
00:02:53,910 --> 00:02:52,560
as 5

94
00:02:55,670 --> 00:02:53,920
times 10 to the minus 3 with respect to

95
00:02:56,869 --> 00:02:55,680
total hydrogen because most hydrogen in

96
00:02:59,509 --> 00:02:56,879
this dark cloud is locked up in

97
00:03:01,030 --> 00:02:59,519
molecular form

98
00:03:02,309 --> 00:03:01,040
okay so i'm not sure how well this is

99
00:03:04,309 --> 00:03:02,319
going to translate i think you can you

100
00:03:05,910 --> 00:03:04,319
can see it there are these dark clouds

101
00:03:07,190 --> 00:03:05,920
here this is just a picture of the night

102
00:03:08,710 --> 00:03:07,200
sky

103
00:03:11,110 --> 00:03:08,720
with a fairly good camera and you can

104
00:03:13,350 --> 00:03:11,120
actually see these dark clouds imprinted

105
00:03:15,750 --> 00:03:13,360
uh on the background field stars so

106
00:03:17,350 --> 00:03:15,760
these are very large regions and you

107
00:03:19,030 --> 00:03:17,360
can't really tell that it's there apart

108
00:03:20,070 --> 00:03:19,040
from the fact that it obscures the stars

109
00:03:21,509 --> 00:03:20,080
behind it

110
00:03:23,509 --> 00:03:21,519
the easiest way to observe what's in

111
00:03:25,270 --> 00:03:23,519
these clouds is to find a reference star

112
00:03:27,509 --> 00:03:25,280
near the edge of one of these clouds and

113
00:03:30,309 --> 00:03:27,519

take spectra of that star and notice how

114
00:03:32,470 --> 00:03:30,319
the stars spectra maybe compare it to an

115
00:03:34,149 --> 00:03:32,480
average star that's not being obscured

116
00:03:37,509 --> 00:03:34,159
and see how that cloud is affecting the

117
00:03:39,830 --> 00:03:37,519
spectra of the background star

118
00:03:42,550 --> 00:03:39,840
so doing this um mostly in the seven

119
00:03:43,830 --> 00:03:42,560
millimeter or the radio

120
00:03:45,270 --> 00:03:43,840
looking at that one i just showed which

121
00:03:47,430 --> 00:03:45,280
is the taurus molecular cloud is kind of

122
00:03:48,710 --> 00:03:47,440
the archetypal molecular cloud

123
00:03:50,470 --> 00:03:48,720
this is just showing you a list of the

124
00:03:51,589 --> 00:03:50,480
gas species greater than some arbitrary

125
00:03:52,949 --> 00:03:51,599
cut off

126
00:03:54,550 --> 00:03:52,959
just to show you that there is a diverse

127
00:03:56,149 --> 00:03:54,560
amount of gas species

128
00:03:58,149 --> 00:03:56,159
there's plenty of aliphatics and or

129
00:03:59,429 --> 00:03:58,159
other just carbon bearing species

130
00:04:00,390 --> 00:03:59,439
there's plenty of nitrogen bearing

131
00:04:02,229 --> 00:04:00,400
species

132
00:04:03,670 --> 00:04:02,239
there's some interesting oxygen variant

133
00:04:05,589 --> 00:04:03,680
species and even one that contains

134
00:04:07,910 --> 00:04:05,599
sulfur although

135
00:04:09,190 --> 00:04:07,920
i generally neglect sulfur because it

136
00:04:11,429 --> 00:04:09,200
doesn't do anything interesting in my

137
00:04:13,350 --> 00:04:11,439
models

138
00:04:15,270 --> 00:04:13,360

and then here is just a large table that

139
00:04:17,030 --> 00:04:15,280
has more information i needed but it was

140
00:04:18,789 --> 00:04:17,040
a good reference so this is for ice

141
00:04:21,349 --> 00:04:18,799
abundances and this is generally done

142
00:04:22,710 --> 00:04:21,359
with infrared band absorption

143
00:04:24,150 --> 00:04:22,720
and the interesting ones i've tried to

144
00:04:26,469 --> 00:04:24,160
highlight you can see this is just

145
00:04:28,870 --> 00:04:26,479
listed as a percentage of water ice and

146
00:04:30,629 --> 00:04:28,880
this ice is forming on dust greens so

147
00:04:32,230 --> 00:04:30,639
this large cloud is mostly gas but it

148
00:04:35,110 --> 00:04:32,240
does contain about a hundredth of its

149
00:04:37,270 --> 00:04:35,120
mass in in dust and this dust is usually

150
00:04:39,350 --> 00:04:37,280
either silicates or carbonaceous

151
00:04:41,430 --> 00:04:39,360
and as this cloud just sits there the

152
00:04:43,749 --> 00:04:41,440
gas species will collapse or collide

153
00:04:45,990 --> 00:04:43,759
with the grain surface you assume some

154
00:04:47,510 --> 00:04:46,000
some sticking parameter and things just

155
00:04:49,590 --> 00:04:47,520
started creating onto the the dust

156
00:04:51,110 --> 00:04:49,600
surfaces and as these things accrete you

157
00:04:54,230 --> 00:04:51,120
know we call them ice

158
00:04:57,430 --> 00:04:54,240
and you can see that uh the first five

159
00:04:59,430 --> 00:04:57,440
uh columns here are protos or stars or

160
00:05:01,350 --> 00:04:59,440
protostars allia 16 is a background

161
00:05:03,590 --> 00:05:01,360
field star for the molecular cloud

162
00:05:05,430 --> 00:05:03,600
whereas these four here are protostars

163
00:05:07,029 --> 00:05:05,440

so that's past the point of quiescence

164
00:05:08,710 --> 00:05:07,039
that's started to collapse and it's the

165
00:05:10,390 --> 00:05:08,720
center has started to heat up

166
00:05:12,710 --> 00:05:10,400
and it started to thermally process the

167
00:05:15,350 --> 00:05:12,720
ice and so co is the most volatile ice

168
00:05:16,950 --> 00:05:15,360
species so it's its uh composition is

169
00:05:19,029 --> 00:05:16,960
decreased the composition of the ice as

170
00:05:21,670 --> 00:05:19,039
co is decreasing you can notice that the

171
00:05:22,870 --> 00:05:21,680
co2 is relatively constant which implies

172
00:05:24,550 --> 00:05:22,880
that it's

173
00:05:27,110 --> 00:05:24,560
a relatively robust mechanism must be

174
00:05:28,310 --> 00:05:27,120
forming co2 in this in these regions

175
00:05:29,510 --> 00:05:28,320
and then the rest that i've highlighted

176
00:05:31,270 --> 00:05:29,520
are just kind of interesting things that

177
00:05:33,749 --> 00:05:31,280
we'll be looking at later in my plots

178
00:05:36,070 --> 00:05:33,759
one particular thing to note is methanol

179
00:05:37,430 --> 00:05:36,080
in the least processed ices there's not

180
00:05:39,110 --> 00:05:37,440
too much methanol

181
00:05:40,390 --> 00:05:39,120
in the kind of intermediate processing

182
00:05:41,670 --> 00:05:40,400
stage there's quite a bit of methanol

183
00:05:43,670 --> 00:05:41,680
it's actually the second most abundant

184
00:05:45,270 --> 00:05:43,680
ice in some protostars and then in the

185
00:05:46,469 --> 00:05:45,280
highly processed protostars where the

186
00:05:47,909 --> 00:05:46,479
the the

187
00:05:49,909 --> 00:05:47,919
cartilage disc is starting to be

188
00:05:51,029 --> 00:05:49,919

evacuated by the heat of the the inner

189
00:05:55,110 --> 00:05:51,039
star

190
00:05:57,270 --> 00:05:55,120
this just points to

191
00:05:59,510 --> 00:05:57,280
high processing either

192
00:06:01,350 --> 00:05:59,520
evacuating the ice off or

193
00:06:03,990 --> 00:06:01,360
supplying sublimating the ice off of the

194
00:06:05,510 --> 00:06:04,000
dust surface or even just

195
00:06:07,510 --> 00:06:05,520
decomposing some of the more complex

196
00:06:09,510 --> 00:06:07,520
species the last column here besides

197
00:06:11,749 --> 00:06:09,520
comets sahaja star is the center of the

198
00:06:13,909 --> 00:06:11,759
galaxy where there is just a large very

199
00:06:16,309 --> 00:06:13,919
interesting molecular cloud that's being

200
00:06:18,830 --> 00:06:16,319
irradiated by many different sources and

201
00:06:20,629 --> 00:06:18,840
so it's kind of an outlier and hard to

202
00:06:26,469 --> 00:06:20,639
model

203
00:06:28,390 --> 00:06:26,479
something that you've probably all done

204
00:06:30,070 --> 00:06:28,400
in say a high school chemistry course

205
00:06:32,150 --> 00:06:30,080
you just have a couple

206
00:06:33,590 --> 00:06:32,160
rate equations for a chemical species to

207
00:06:36,629 --> 00:06:33,600
evolve or to react with some other

208
00:06:37,909 --> 00:06:36,639
chemical species to form another one

209
00:06:39,510 --> 00:06:37,919
and then you have you know instead of

210
00:06:41,590 --> 00:06:39,520
one of those you have 12 000 reactions

211
00:06:43,749 --> 00:06:41,600
now and they're all coupled

212
00:06:46,469 --> 00:06:43,759
with 1200 separate chemical species

213
00:06:48,309 --> 00:06:46,479

reacting using 12 elements

214
00:06:50,150 --> 00:06:48,319
you have to specify those in local

215
00:06:51,830 --> 00:06:50,160
environmental parameters again and you

216
00:06:53,350 --> 00:06:51,840
evolve what's initially an atomic gas

217
00:06:55,110 --> 00:06:53,360
with the exception of molecular hydrogen

218
00:06:57,110 --> 00:06:55,120
generally just through time just letting

219
00:06:58,710 --> 00:06:57,120
the reaction network do its thing so you

220
00:07:00,629 --> 00:06:58,720
know most reactions here are not going

221
00:07:02,629 --> 00:07:00,639
to have a barrier because there's enough

222
00:07:03,749 --> 00:07:02,639
reactions that if anything has a barrier

223
00:07:05,589 --> 00:07:03,759
it's probably just going to be safely

224
00:07:07,189 --> 00:07:05,599
ignored all gas phase reactions

225
00:07:08,870 --> 00:07:07,199
essentially are barrier-less the

226
00:07:11,110 --> 00:07:08,880
solid-state reactions can have a barrier

227
00:07:13,430 --> 00:07:11,120
and that gets a little more complex

228
00:07:15,110 --> 00:07:13,440
it is a three-phase model so we

229
00:07:16,710 --> 00:07:15,120
worry about gas species we worry about

230
00:07:18,629 --> 00:07:16,720
the accretion of the gas species onto a

231
00:07:20,469 --> 00:07:18,639
grain surface you have grain surface

232
00:07:22,390 --> 00:07:20,479
reactions and then you have an ice

233
00:07:25,110 --> 00:07:22,400
mantle where more reactions can occur

234
00:07:26,629 --> 00:07:25,120
but you can also just sequester species

235
00:07:28,390 --> 00:07:26,639
you can kind of imagine how this model

236
00:07:30,550 --> 00:07:28,400
works it is not spatial whatsoever it is

237
00:07:33,270 --> 00:07:30,560
a 0d model it is just essentially a

238
00:07:34,790 --> 00:07:33,280

chemistry accounting model

239
00:07:36,230 --> 00:07:34,800
but you can imagine how we treat the

240
00:07:39,589 --> 00:07:36,240
grain surface is kind of just like a

241
00:07:40,469 --> 00:07:39,599
golf ball um you we assign the dust

242
00:07:42,390 --> 00:07:40,479
grain to have a certain amount of

243
00:07:44,230 --> 00:07:42,400
binding sites in this case roughly a

244
00:07:45,350 --> 00:07:44,240
million for a typical grain size of 0.1

245
00:07:47,110 --> 00:07:45,360
micron

246
00:07:48,710 --> 00:07:47,120
and as a species of creates onto the

247
00:07:51,350 --> 00:07:48,720
surface it sticks into a dimple of the

248
00:07:53,029 --> 00:07:51,360
golf ball and then it has two barriers

249
00:07:54,710 --> 00:07:53,039
to either diffuse around the surface

250
00:07:56,790 --> 00:07:54,720
through the dimples or a barrier to just

251
00:07:58,390 --> 00:07:56,800
pop off the grain and desorb back into

252
00:07:59,990 --> 00:07:58,400
the gas phase

253
00:08:01,510 --> 00:08:00,000
and then as things accrete you

254
00:08:04,710 --> 00:08:01,520
essentially just layer things on top of

255
00:08:06,150 --> 00:08:04,720
each other and the ice mantle grows

256
00:08:09,110 --> 00:08:06,160
and i just have a list of included

257
00:08:10,790 --> 00:08:09,120
reactions if people like chemistry um

258
00:08:12,390 --> 00:08:10,800
but it's essentially just out of those

259
00:08:14,469 --> 00:08:12,400
12 000 reactions you're going to have

260
00:08:15,909 --> 00:08:14,479
some cosmic ray

261
00:08:21,110 --> 00:08:15,919
interesting reactions some

262
00:08:22,710 --> 00:08:21,120
photoionization ions neutrals etc etc

263
00:08:25,350 --> 00:08:22,720

so all that's kind of the background the

264
00:08:27,589 --> 00:08:25,360
thing that i'm adding to to the field or

265
00:08:29,350 --> 00:08:27,599
attempting to um maybe modifying some

266
00:08:32,550 --> 00:08:29,360
other work is to add this grain size

267
00:08:34,469 --> 00:08:32,560
distribution um so the almost all prior

268
00:08:36,630 --> 00:08:34,479
models the exception of one has assumed

269
00:08:39,029 --> 00:08:36,640
a canonical grain size um it's just kind

270
00:08:40,870 --> 00:08:39,039
of a necessary thing especially earlier

271
00:08:43,990 --> 00:08:40,880
with you know numerical models in the

272
00:08:45,829 --> 00:08:44,000
70s 80s 90s you can't do too much and so

273
00:08:47,190 --> 00:08:45,839
an easy simplification was assume all

274
00:08:49,190 --> 00:08:47,200
grains are the same size and that they

275
00:08:51,030 --> 00:08:49,200
don't grow so you just leave it at 0.1

276
00:08:53,750 --> 00:08:51,040
micron but of course in reality that's

277
00:08:56,710 --> 00:08:53,760
not true and we want to investigate what

278
00:08:59,110 --> 00:08:56,720
might change if we were to uh involve

279
00:09:01,030 --> 00:08:59,120
this or invoke this distribution so how

280
00:09:03,269 --> 00:09:01,040
do we find it well again we just use our

281
00:09:05,670 --> 00:09:03,279
extinction curve we find this background

282
00:09:08,630 --> 00:09:05,680
field star we find a model spectra for a

283
00:09:10,630 --> 00:09:08,640
star like that uh for a star of similar

284
00:09:13,430 --> 00:09:10,640
character and then we find how it's

285
00:09:15,110 --> 00:09:13,440
extincted by this cloud

286
00:09:17,509 --> 00:09:15,120
and most of this this extinction is just

287
00:09:20,150 --> 00:09:17,519
occurring due to dust and an individual

288
00:09:22,310 --> 00:09:20,160

dust grain of a given size will remove

289
00:09:23,829 --> 00:09:22,320
will absorb light of given wavelengths

290
00:09:25,990 --> 00:09:23,839
in a certain pattern there's plenty of

291
00:09:27,430 --> 00:09:26,000
theory for this me theory or just if

292
00:09:29,990 --> 00:09:27,440
your grain is small or large enough you

293
00:09:32,550 --> 00:09:30,000
get into rayleigh limit or just

294
00:09:34,710 --> 00:09:32,560
black body limits

295
00:09:35,990 --> 00:09:34,720
someone did this in 1977 and i just used

296
00:09:37,350 --> 00:09:36,000
his model because it's the most

297
00:09:39,030 --> 00:09:37,360
straightforward it's the easiest way to

298
00:09:40,470 --> 00:09:39,040
just throw it in my chemical model and

299
00:09:42,710 --> 00:09:40,480
see what happens

300
00:09:44,070 --> 00:09:42,720
and his model just uses a power law for

301
00:09:45,750 --> 00:09:44,080
the distribution

302
00:09:48,389 --> 00:09:45,760
of how how many grains you expect for a

303
00:09:50,550 --> 00:09:48,399
given size here a is the radius so the

304
00:09:53,509 --> 00:09:50,560
number of grains per given radius

305
00:09:55,190 --> 00:09:53,519
goes as the radius to the minus 3.5

306
00:09:57,269 --> 00:09:55,200
this is um

307
00:09:58,790 --> 00:09:57,279
i guess what this tells you is that if

308
00:10:00,710 --> 00:09:58,800
you were to plot the total amount of

309
00:10:02,310 --> 00:10:00,720
cross-sectional area for a given size of

310
00:10:04,150 --> 00:10:02,320
grain that the total amount of

311
00:10:05,910 --> 00:10:04,160
cross-sectional area goes up as you go

312
00:10:07,990 --> 00:10:05,920
to smaller grains and this is going to

313
00:10:08,949 --> 00:10:08,000

be important because the grain surface

314
00:10:10,790 --> 00:10:08,959
is where a lot of the interesting

315
00:10:12,790 --> 00:10:10,800
chemistry occurs and for chemistry to

316
00:10:14,870 --> 00:10:12,800
occur on the grain surface gas species

317
00:10:16,389 --> 00:10:14,880
need to accrete onto that grain surface

318
00:10:17,750 --> 00:10:16,399
and if the small grains have the largest

319
00:10:19,509 --> 00:10:17,760
cross-sectional area they're going to be

320
00:10:20,710 --> 00:10:19,519
accreting the most gas and therefore

321
00:10:22,389 --> 00:10:20,720
will be affecting the chemistry the

322
00:10:23,990 --> 00:10:22,399
strongest

323
00:10:26,389 --> 00:10:24,000
okay so the goal now is to find the

324
00:10:27,190 --> 00:10:26,399
effect of this distribution

325
00:10:29,430 --> 00:10:27,200
so

326
00:10:31,030 --> 00:10:29,440
how do you at least initially might

327
00:10:33,509 --> 00:10:31,040
expect this grain distribution to affect

328
00:10:35,350 --> 00:10:33,519
the model well one you might expect as

329
00:10:36,710 --> 00:10:35,360
the grains grow

330
00:10:38,069 --> 00:10:36,720
and have different sizes you might

331
00:10:39,829 --> 00:10:38,079
expect that the total number of binding

332
00:10:41,430 --> 00:10:39,839
sites on the surface might play a role

333
00:10:43,829 --> 00:10:41,440
so the first model here is just a single

334
00:10:45,430 --> 00:10:43,839
grain size the control model and the

335
00:10:47,670 --> 00:10:45,440
next model that i ran is just five

336
00:10:49,590 --> 00:10:47,680
grains but with uniform temperature and

337
00:10:51,110 --> 00:10:49,600
so this is just to find the effect of

338
00:10:53,509 --> 00:10:51,120

how the different grain sizes might

339
00:10:55,590 --> 00:10:53,519
change the chemistry the next thing way

340
00:10:56,870 --> 00:10:55,600
you might expect the grains to matter

341
00:10:58,069 --> 00:10:56,880
the different grain sizes to matter is

342
00:10:59,350 --> 00:10:58,079
that

343
00:11:02,389 --> 00:10:59,360
if you have a different grain size you

344
00:11:03,750 --> 00:11:02,399
might absorb and emit uh absorb or emit

345
00:11:04,630 --> 00:11:03,760
energy in different manners and

346
00:11:05,670 --> 00:11:04,640
therefore might have different

347
00:11:07,430 --> 00:11:05,680
temperatures

348
00:11:08,870 --> 00:11:07,440
and a kind of a canonical estimate on

349
00:11:10,069 --> 00:11:08,880
how these different grains might have

350
00:11:11,829 --> 00:11:10,079
different temperatures is just another

351
00:11:13,430 --> 00:11:11,839
simple power law astronomers love power

352
00:11:14,949 --> 00:11:13,440
laws and this power realized that the

353
00:11:16,470 --> 00:11:14,959
temperature of a grain might go as the

354
00:11:18,150 --> 00:11:16,480
or should go as the radius of the grain

355
00:11:19,590 --> 00:11:18,160
to the minus one sixth so the smaller

356
00:11:21,030 --> 00:11:19,600
grain should be warmer

357
00:11:22,870 --> 00:11:21,040
so this is a five grain plot

358
00:11:24,550 --> 00:11:22,880
distribution um with a distribution of

359
00:11:25,829 --> 00:11:24,560
both size and temperature i'll explain

360
00:11:27,350 --> 00:11:25,839
how these plots work real quick and then

361
00:11:29,190 --> 00:11:27,360
this last one is just a collapse model

362
00:11:30,630 --> 00:11:29,200
so it's not a quiescent cloud but

363
00:11:31,910 --> 00:11:30,640

collapse models generally try and

364
00:11:32,870 --> 00:11:31,920
represent

365
00:11:35,509 --> 00:11:32,880
actual

366
00:11:36,710 --> 00:11:35,519
physical conditions a bit more precisely

367
00:11:39,030 --> 00:11:36,720
so what i'm showing here is just the

368
00:11:41,030 --> 00:11:39,040
radius on the left and the radius is the

369
00:11:42,790 --> 00:11:41,040
dashed lines and the right is the

370
00:11:44,710 --> 00:11:42,800
temperature with the solid lines and so

371
00:11:47,509 --> 00:11:44,720
just how these evolve through my model

372
00:11:49,670 --> 00:11:47,519
time on the x-axis so we go from we

373
00:11:51,910 --> 00:11:49,680
essentially do a model for 10 million

374
00:11:53,990 --> 00:11:51,920
years and you can see that

375
00:11:56,389 --> 00:11:54,000
the grains grow in all models the dash

376
00:11:58,870 --> 00:11:56,399
lines do do increase the size is here

377
00:12:01,350 --> 00:11:58,880
this is a micron

378
00:12:03,910 --> 00:12:01,360
so for a single grain size the the mean

379
00:12:06,069 --> 00:12:03,920
grain size is is roughly a micron um

380
00:12:07,509 --> 00:12:06,079
whereas here we you can see that

381
00:12:09,350 --> 00:12:07,519
oh sorry this is in centimeters that's

382
00:12:11,430 --> 00:12:09,360
that's smaller than a micron that's uh

383
00:12:12,710 --> 00:12:11,440
it raises to about 0.1 micron

384
00:12:14,230 --> 00:12:12,720
but here you can see these grains are

385
00:12:17,030 --> 00:12:14,240
growing but i fixed the temperature this

386
00:12:19,030 --> 00:12:17,040
is just to kind of disentangle the

387
00:12:20,470 --> 00:12:19,040
the uh the number of great binding sites

388
00:12:22,310 --> 00:12:20,480

versus the temperature effects and here

389
00:12:24,069 --> 00:12:22,320
you can see that the temperatures are

390
00:12:25,990 --> 00:12:24,079
evolved through my static model they

391
00:12:28,550 --> 00:12:26,000
actually decrease and that's because as

392
00:12:29,829 --> 00:12:28,560
these ice mantles grow these grains are

393
00:12:31,990 --> 00:12:29,839
essential their effective area is

394
00:12:33,590 --> 00:12:32,000
increasing and because the temperature

395
00:12:34,790 --> 00:12:33,600
is determined by the size of the grain

396
00:12:36,389 --> 00:12:34,800
as the grains are growing their

397
00:12:37,910 --> 00:12:36,399
temperature is lowering and so you can

398
00:12:39,670 --> 00:12:37,920
see that for the smallest grains that

399
00:12:41,990 --> 00:12:39,680
start at roughly 15 and a half kelvin

400
00:12:42,790 --> 00:12:42,000
they end below 13.

401
00:12:45,190 --> 00:12:42,800
so

402
00:12:46,790 --> 00:12:45,200
now we'll get into the actual chemistry

403
00:12:48,949 --> 00:12:46,800
this is just a representative plot of

404
00:12:50,389 --> 00:12:48,959
the single grain control model this is

405
00:12:52,389 --> 00:12:50,399
water at the top water is always the

406
00:12:55,829 --> 00:12:52,399
most dominant ice species so i know that

407
00:12:56,710 --> 00:12:55,839
that's getting that's doing a decent job

408
00:12:59,190 --> 00:12:56,720
here

409
00:13:01,350 --> 00:12:59,200
the magenta is methanol with blue as

410
00:13:03,269 --> 00:13:01,360
formaldehyde and methanol is a product

411
00:13:05,350 --> 00:13:03,279
of formaldehyde and so they should trail

412
00:13:06,949 --> 00:13:05,360
each other fairly well which they do

413
00:13:09,190 --> 00:13:06,959

red is carbon monoxide and green is

414
00:13:11,110 --> 00:13:09,200
carbon dioxide and the two dash species

415
00:13:12,230 --> 00:13:11,120
are just hydrogenated species which we

416
00:13:13,590 --> 00:13:12,240
don't like to care about because they're

417
00:13:14,949 --> 00:13:13,600
not interesting they don't do much other

418
00:13:17,430 --> 00:13:14,959
than just

419
00:13:19,350 --> 00:13:17,440
abstract hydrogen

420
00:13:21,750 --> 00:13:19,360
so here you can see that for a single

421
00:13:24,470 --> 00:13:21,760
grain i have mostly carbon monoxide of

422
00:13:25,990 --> 00:13:24,480
the two carbon and oxygen species

423
00:13:27,110 --> 00:13:26,000
now getting into the next model which is

424
00:13:28,710 --> 00:13:27,120
where it gets complicated to try and

425
00:13:30,470 --> 00:13:28,720
show this i essentially have an

426
00:13:32,710 --> 00:13:30,480
aggregate mantle this is for the five

427
00:13:34,310 --> 00:13:32,720
grains with the uniform temperature this

428
00:13:35,509 --> 00:13:34,320
is the aggregate ice mantle add up all

429
00:13:37,030 --> 00:13:35,519
the ice mantels off the five different

430
00:13:39,190 --> 00:13:37,040
grain sizes this is the mantle for the

431
00:13:41,509 --> 00:13:39,200
smallest grain the medium grain and the

432
00:13:43,509 --> 00:13:41,519
fifth grain and you can see if i flip

433
00:13:45,190 --> 00:13:43,519
back and forth here um just the general

434
00:13:46,790 --> 00:13:45,200
shapes of these of these plots look

435
00:13:48,710 --> 00:13:46,800
roughly the same

436
00:13:50,470 --> 00:13:48,720
and i can show that at the end that the

437
00:13:52,470 --> 00:13:50,480
the total chemistry doesn't change

438
00:13:53,829 --> 00:13:52,480

appreciably between those two models so

439
00:13:55,030 --> 00:13:53,839
the grain distribution doesn't really do

440
00:13:57,350 --> 00:13:55,040
much if i don't have a temperature

441
00:13:59,750 --> 00:13:57,360
distribution but now if i go from these

442
00:14:01,829 --> 00:13:59,760
plots to a distribution and temperature

443
00:14:02,870 --> 00:14:01,839
as you may expect just even naively that

444
00:14:04,069 --> 00:14:02,880
a temperature distribution probably is

445
00:14:05,509 --> 00:14:04,079
going to affect the chemistry because

446
00:14:06,550 --> 00:14:05,519
the temperature is what determines how

447
00:14:08,790 --> 00:14:06,560
my rates

448
00:14:09,990 --> 00:14:08,800
are how my reactions move right if a

449
00:14:10,790 --> 00:14:10,000
rate constant

450
00:14:12,629 --> 00:14:10,800
uh

451
00:14:14,470 --> 00:14:12,639
well generally you know chemical rates

452
00:14:16,150 --> 00:14:14,480
depend on the temperature and here the

453
00:14:19,350 --> 00:14:16,160
big chemical rate that's important here

454
00:14:21,670 --> 00:14:19,360
is the conversion of co2 co2 through

455
00:14:23,910 --> 00:14:21,680
various rates um is the most temperature

456
00:14:25,189 --> 00:14:23,920
sensitive in the region of 10 kelvin so

457
00:14:26,790 --> 00:14:25,199
for a temperature distribution that i

458
00:14:28,790 --> 00:14:26,800
showed earlier where the grains have a

459
00:14:30,150 --> 00:14:28,800
temperature between 9 and 15 kelvin

460
00:14:32,949 --> 00:14:30,160
there's a transitionary temperature

461
00:14:35,189 --> 00:14:32,959
around 10 around 12 kelvin where co

462
00:14:36,710 --> 00:14:35,199
becomes efficiently converted into co2

463
00:14:38,230 --> 00:14:36,720

and so here for my smallest grain of

464
00:14:39,990 --> 00:14:38,240
distribution temperature you can see

465
00:14:42,629 --> 00:14:40,000
that the co2 is actually competing with

466
00:14:44,550 --> 00:14:42,639
water for um an immense amount of ice

467
00:14:46,629 --> 00:14:44,560
formation whereas co has dropped off the

468
00:14:49,269 --> 00:14:46,639
radar until the grain gets sufficiently

469
00:14:51,110 --> 00:14:49,279
large to cool off that co becomes uh

470
00:14:53,509 --> 00:14:51,120
competitive in the reaction rates again

471
00:14:54,949 --> 00:14:53,519
and even in the aggregate ice mantle co2

472
00:14:57,350 --> 00:14:54,959
is dominant because the smallest grain

473
00:14:58,470 --> 00:14:57,360
is excreting the most ice

474
00:15:01,110 --> 00:14:58,480
here's the collapse i'm just going to

475
00:15:02,550 --> 00:15:01,120
skip it because i'm running low

476
00:15:04,389 --> 00:15:02,560
so this is just the table that shows

477
00:15:05,910 --> 00:15:04,399
that the single grain model is very

478
00:15:07,189 --> 00:15:05,920
comparable to the five grain model with

479
00:15:08,629 --> 00:15:07,199
uniform temperature you can just compare

480
00:15:10,470 --> 00:15:08,639
all the numbers they're all about the

481
00:15:11,750 --> 00:15:10,480
same the difference here comes with the

482
00:15:13,990 --> 00:15:11,760
temperature difference there's less

483
00:15:15,189 --> 00:15:14,000
water ice because the the warmer grains

484
00:15:16,949 --> 00:15:15,199
essentially are

485
00:15:18,870 --> 00:15:16,959
allow water to more easily absorb off

486
00:15:21,350 --> 00:15:18,880
the surface and also the amount of co

487
00:15:22,949 --> 00:15:21,360
has dropped the amount of co2 has grown

488
00:15:24,310 --> 00:15:22,959

the amount of methanol has also dropped

489
00:15:25,110 --> 00:15:24,320
and that's kind of a curious thing

490
00:15:26,389 --> 00:15:25,120
because

491
00:15:27,990 --> 00:15:26,399
you might expect that

492
00:15:29,750 --> 00:15:28,000
methanol would grow just because warmer

493
00:15:31,910 --> 00:15:29,760
temperatures maybe is makes more complex

494
00:15:33,030 --> 00:15:31,920
species more easily formable but

495
00:15:35,350 --> 00:15:33,040
methanol generally requires

496
00:15:37,110 --> 00:15:35,360
hydrogenation of co and if cos being

497
00:15:39,509 --> 00:15:37,120
formed into co2

498
00:15:41,350 --> 00:15:39,519
the formation of methanol is inhibited

499
00:15:42,790 --> 00:15:41,360
so just a quick conclusion slide i guess

500
00:15:44,629 --> 00:15:42,800
i've probably talked about most of this

501
00:15:51,189 --> 00:15:44,639
so you can just read them out of time

502
00:15:51,199 --> 00:16:02,310
we have time for one quick question

503
00:16:05,990 --> 00:16:04,310
do you allow for bulk diffusion in your

504
00:16:07,189 --> 00:16:06,000
grain model and if so what's your bulk

505
00:16:09,110 --> 00:16:07,199
diffusion

506
00:16:11,189 --> 00:16:09,120
yes right yeah so

507
00:16:13,269 --> 00:16:11,199
as the ice species uh get sequestered

508
00:16:14,870 --> 00:16:13,279
into the mantle a lot of previous models

509
00:16:16,629 --> 00:16:14,880
would just say the ice is now completely

510
00:16:17,749 --> 00:16:16,639
dormant and nothing occurs and they just

511
00:16:19,749 --> 00:16:17,759
build up and then you can look at the

512
00:16:21,430 --> 00:16:19,759
ice at the end the small does include

513
00:16:23,110 --> 00:16:21,440

bulk diffusion and so you can allow

514
00:16:24,629 --> 00:16:23,120
these ice species even while in the

515
00:16:27,430 --> 00:16:24,639
mantle and not no longer on the surface

516
00:16:28,949 --> 00:16:27,440
to react with other ice species um it

517
00:16:30,790 --> 00:16:28,959
does ends up not playing a huge role in

518
00:16:32,550 --> 00:16:30,800
this model but if the temperature were

519
00:16:34,710 --> 00:16:32,560
say double to around 20 kelvin maybe in

520
00:16:36,629 --> 00:16:34,720
a warm-up stage of a protostar that can

521
00:16:38,550 --> 00:16:36,639
become very important um but for this