



分子云天体化学模型的进展

葛继兴^{1,2*}, 蔡文仲^{4,5,1}, 张霞^{1,2,3}, 李芳芳^{1,2}, 王晶晶⁵

1. 中国科学院新疆天文台, 乌鲁木齐 830011

2. 新疆射电天体物理重点实验室, 乌鲁木齐 830011

3. 射电天文与技术重点实验室(中国科学院), 北京 100101

4. 中国石油大学(北京)理学院, 北京 102200

5. 中国石油大学(北京)克拉玛依校区文理学院, 克拉玛依 834000

* 联系人, E-mail: gejixing@xao.ac.cn

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摘要 天体化学是一门天文、物理与化学的交叉性前沿学科, 其结合了天文观测、实验室化学与数值模拟等方面, 在几十年来成果丰硕. 天体化学模型作为其中的一个主要方面, 在人们理解星际分子云中分子的物理和化学形成机制上起到关键作用. 本文介绍了天体化学模型的发展过程、数值模拟方法与程序, 探讨了在物理和化学机制方面取得的最新进展. 本文对天体化学模型的数值方法、天体化学数据库和数值模拟程序等基础方面进行了介绍, 并着重介绍了速率方程方法和蒙特卡罗数值方法的基本原理. 结合天文观测数据, 以典型代表性分子为例(如CO、NH₃、OCS和有机分子等), 本文阐述了天体化学模型在分子吸附和解吸附、硫元素的主要分子形式和尘埃冰成分, 以及复杂有机分子形成等方面取得的成果和不足. 以典型分子云TMC-1中丰富的分子观测丰度数据为观测分子的样本, 本文将其与包含有同位素分子的天体化学模型结果进行了比较, 展示了模型与观测之间的符合度, 并探讨了观测与模型间存在的差异和提升空间. 最后, 本文探讨了机器学习在天体化学模型方面的发展与应用. 随着天文观测技术和设备的不断升级、模型和数值计算算法的不断更新, 以及实验室测量数据的不断完善, 分子云内天体化学模型的研究将迎来很大发展.

关键词 天体化学, 分子云, 分子丰度, 数值模拟

分子云作为恒星形成的初始阶段, 其物理性质(密度 $n_{\text{H}} \sim 10^4 \text{ cm}^{-3}$, 温度 $T \sim 10 \text{ K}$, 消光 $A_{\text{V}} \sim 10 \text{ mag}$)^[1]为分子的形成提供了条件, 特别是为复杂有机分子在尘埃表面和冰内的形成提供了场所^[2,3]. 分子谱线作为物理和化学信息的载体, 是人们研究分子云的基本手段. 截至目前(2024年11月), 已有超过 320 种分子在不同物理环境中被观测到, 其中包括简单的分子、离子、复杂的有机分子等(<https://cdms.astro.uni-koeln.de/classic/molecules>), 为人类研究

分子的形成过程提供了观测的关键证据.

天体化学作为一门交叉性前沿学科, 不同于专注于物理性质(气体密度、温度、分子谱线强度、轮廓、分布、丰度等)的天体物理的研究, 它通过分子的化学性质来研究天文环境中分子的化学形成过程, 进而与物理性质相耦合, 共同形成对目标天体的限制. 天体化学结合了天文观测、实验室测量、量子化学计算和天体化学数值模拟等内容, 在物理和化学两个方面, 相互耦合、限制和验证, 不断推动着对目标天体的科学认知.

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基于星际物质主要有两种形态(即气体和尘埃),天体化学数值模拟逐步发展. 真正意义上的两相(气体+尘埃)的天体化学模型于1992年发布^[4], 随后又在各个方面做了大量改进且发展成为三相模型(气体+尘埃表面+尘埃冰壳层)^[5,6]. 近30年来, 天体化学模型得到了持续的发展, 为天文观测的现象提供了新的解释, 但也存在着一些不足. 本文以分子云为例, 主要探讨天体化学模型的新进展, 并对目前存在的问题加以讨论.

1 化学过程数值建模

由于星际环境的密度较低, 三体化学反应发生的概率很低, 大多数化学反应均为两体化学反应^[2]. 主流的天体化学模型框架下, “气体+尘埃”的化学模型被人们广泛使用, 即分子既在气相化学反应中产生和消耗, 同时在尘埃(固相)上也发生丰富的化学过程. 气相和固相通过吸附和解吸附过程进行物质的交换. 在不同的物理环境下, 发生的化学过程不尽相同, 从而产生了分子在天文射电波段不同的观测性质(如谱线轮廓的多样性, 丰度大小、空间分布情况等). 可见, 天体化学建模对理解星际空间的化学过程起到至关重要的作用.

1.1 速率方程

通过求解基于速率方程的分子相关的刚性微分方程组, 可以得到分子密度随时间的演化. 一般的两相模型(气相+尘埃表面)的化学过程, 需要求解以下方程^[4,7]:

$$\frac{dn_i}{dt} = \sum_{j,l} k_{j,l} n_j n_l - \sum_{i,h} k_{i,h} n_i n_h - k_{acc} n_i + k_{des} n_i^s, \quad (1)$$

$$\frac{dn_i^s}{dt} = \sum_{j,k} k_{j,k} n_j n_k^s - \sum_{i,l} k_{i,l} n_i^s n_l^s + k_{acc} n_i - k_{des} n_i^s, \quad (2)$$

其中, n_i 和 n_i^s 分别代表气相和尘埃表面分子 i 的密度, k 代表反应速率系数. 以上分别包含了气相和尘埃表面中分子的产生和消耗过程, 其中也考虑了气相和尘埃间分子的交互过程, 即吸附(accretion)和解吸附(desorption)过程.

考虑 H_2 分子在尘埃上形成, 并忽略吸附和解吸附过程, 即只考虑方程(1)的气相相关部分, 两相模型退化为纯气相模型.

三相模型进一步考虑了尘埃冰表面以下的冰壳层内(图1)的化学过程^[5,6]. 其过程用以下方程描述:

$$\begin{aligned} \frac{dn_i^s}{dt} = & \sum_{j,k} k_{j,k} n_j^m n_k^m - \sum_{i,l} k_{i,l} n_i^m n_l^m + k_{swap}^m n_i^s \\ & - k_{swap}^m n_i^m + \frac{dn_i^s}{dt} |_{s \rightarrow m} - \frac{dn_i^m}{dt} |_{m \rightarrow s}, \end{aligned} \quad (3)$$

其中, 上标“m”代表冰壳层(mantle)分子. k_{swap}^m 是表面与壳层分子间的交换率(swapping rate). 最后两项代表考虑单个分子在表面与壳层间的迁移过程.

与速率方程方法相比较, 下文将提到的蒙特卡罗方法更接近于真实发生在尘埃冰内的微观化学过程, 但该方法计算上却比较耗时. 为了在保证速率方程效率的前提下, 又满足其精度, “修正速率方程的方法”被多位研究者提出^[8~10], 且达到了与蒙特卡罗方法不错的符合度, 这里不再展开叙述.

1.2 蒙特卡罗

1976年, Gillespie^[11]提出了用蒙特卡罗方法数值模拟化学动力学的一般方法, 并验证了其可行性. 由于星际尘埃相关的化学均为微观过程, 因此蒙特卡罗方法相对于速率方程方法更为接近真实的情况, 在天文领域逐步发展起来^[12~14, 23~28]. 蒙特卡罗模型方法的发展也经历了与速率方程方法类似的过程, 人们首先在尘埃表面验证其微观过程的性质和影响^[14, 29~31], 之后

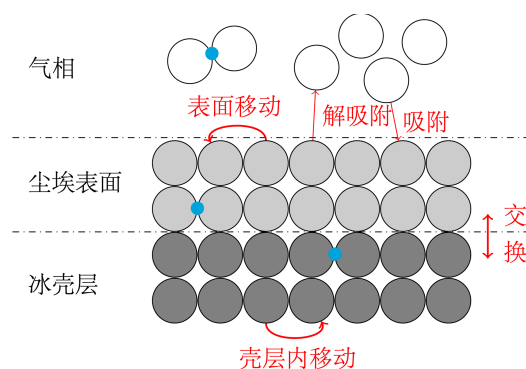


图1 (网络版彩色)三相模型示意图. 空心、灰色和深灰色小球分别代表气相、尘埃表面和冰壳层内的分子(层数仅作为示意). 红色箭头标注典型的过程. 青色实心点标记可能的化学反应(随机)

Figure 1 (Color online) Diagram of the three-phase model. The empty, gray and dark gray balls indicate the gas-phase, dust surface and mantle species, respectively. The number of layers is for illustration purposes only. The red arrows indicate typical processes. The cyan filled points indicate possible reactions (randomly)

才将气体和尘埃加以综合性地考虑,形成了同时考虑了“气体(宏观)+尘埃(微观)”的整合模型^[23~25,27,32]。

在宏观气体层面,需要产生0 ~ 1之间的随机数 R' 来确定第 i 个反应的等待时间(waiting time, $\tau'_i = -\ln(R')/r_i$),进而找到时间最小的反应来发生,并对应地更新相关联分子的丰度即可^[23,24,27]。

在微观尘埃层面,需要考虑尘埃上的位点的网格化(单个尘埃上有 $N = 1.88 \times 10^6$ 个位点,可用矩形网格 $L \times L = N$ 来描述^[23,24]),以及尘埃相关的化学过程(如吸附、解吸附以及尘埃位点上的化学反应)。每一个化学过程都可以当作单独的随机事件来处理,因此需要产生多个随机数($R_{n,n=1,2,3,\dots}$)来确定每一个事件的发生。最终一个事件发生的时间步长,由所有事件中时标最小的事件决定($\tau_{\min} = \min(\tau_{n,n=1,2,3,\dots})$),并对应更新相关联的所有的性质。这里由于篇幅所限,不做具体展开,详见参考文献^[23~25,27,32]。

区别于速率方程方法所采用的单位体积(V_0),在整合的“气体+尘埃”蒙特卡罗化学模型中,除了要整体考虑所有气体和尘埃相关事件中最短的时标外($\tau_{\min} = \min(\tau_{n,n=1,2,3,\dots}, \tau')$),还需要对所考虑的空间体积进行调整($V_0 \rightarrow V_1$),使得尘埃的个数等于1,即^[27]

$$V_1 = \frac{4/3\pi\rho_{\text{dust}}a^3}{\rho_{\text{gas}}R_{\text{d2g}}}, \quad (4)$$

其中, a , ρ_{dust} , ρ_{gas} 和 R_{d2g} 分别为尘埃的半径、尘埃的密度、气体的密度和尘埃与气体的质量比。在实际的模拟过程中,通常采用部分网格进行模拟后,再将模拟的数据调整到真实的情况,这里可以节约一定的计算资源^[24,25]。

使用蒙特卡罗数值模拟方法,多种涉及微观过程的物理化学性质被研究,如 H_2 的形成^[29,30,33]、光

子对不同尺寸尘埃的随机加热所引起的温度波动效应^[33,34],以及复杂有机分子的形成^[24~26]。以上均显示出了尘埃相关的微观过程对分子丰度的重要性。

1.3 模拟程序

基于速率方程的化学模拟程序一直在发展中,新的方法和机制不断引入其中,这使得其存在多个分支。根据科研的需求和目标,不同的程序可适应不同的物理和化学条件,满足不同的科研目的。表1列出了公开发表的基于速率方程的数值模拟程序,并给出了链接。针对纯气相模型开发的数值模拟程序rate13_dc和Nahoon可以分别在天体化学数据库UMIST Udfa (<https://umistdatabase.uk/>或者<https://udfa.ajmarkwick.net>)和KIDA(<https://kida.astrochem-tools.org/>)中获取。针对两相或者三相的模型,数值模型程序有: NAUTILUS, ALCHEMIC^[7], CHEMPL^[35], KROME^[36], GGCHEMPY^[37]等。

在上述模拟程序之中,rate13_dc和Nahoon尽管为纯气相模拟程序,但在测试新的气相化学反应方面具有更加简洁高效的优点,可以避免尘埃相关反应的影响。NAUTILUS, ALCHEMIC和KROME为起步较早的模拟程序,且是较为完善的“气体+尘埃”化学模拟程序,在世界各地科研院所和高校中有着广泛的应用,其成果也是丰富多样的。而CHEMPL和GGCHEMPY为最近几年内公开发表的“气体+尘埃”模型,虽未广泛流行,但凭借其简洁和高效的特点,使用群体数量也开始逐步提升。使用以上模拟程序的科研成果均可在各自的官网(链接见表1)上找到,这里不再罗列。考虑到上述模型大部分使用了Fortran或者C/C++/C# 语言进行编写,虽然保证了效率,但使用的简便度上稍有不足,因此各

表1 基于速率方程的化学模拟程序

Table 1 The rate equation based chemical numerical codes

名称	功能	链接
rate13_dc	纯气相	http://www.udfa.ajmarkwick.net/downloads/rate13_dc.code.tgz
Nahoon	纯气相	https://kida.astrochem-tools.org/codes.html
Astrochem	气相+吸附和解吸附	https://astrochem.readthedocs.io/en/latest/index.html
NAUTILUS	气体+尘埃	https://forge.oas.u-bordeaux.fr/LAB/astrochem-tools/pnautilus
ALCHEMIC	气体+尘埃	https://www2.mpi-hd.mpg.de/homes/semenov/Chemistry_benchmark/codes.html
chempl	气体+尘埃	https://github.com/fjdu/chempl
UCLCHEM	气体+尘埃	https://github.com/uclchem/UCLCHEM
Krome	气体+尘埃	http://kromepackage.org/
GGCHEMPY	气体+尘埃	https://github.com/JixingGE/GGCHEMPY

个模拟程序本身也会提供一些Python语言的接口, 或者脚本, 以方便模型的编译、运行和分析. 在这一方面, 纯Python版本的模拟程序更占优势, 更适合于快速进行科学的尝试, 也更适合于初学者或者教学使用. 这里需指出, 读者应关注化学模拟程序所需的化学反应网络和速率系数的更新, 及时查看UMIST udfa 和KIDA数据库, 以便获取最新的研究成果和推进新的研究.

随着计算机语言的发展, 用于编写模拟程序的语言也在逐步更迭, Fortran和C/C++以其高速的执行效率一直处于主流地位. 未来, 随着计算机能力和计算语言的发展, 结合人工智能机器学习等算法, 天体化学数值计算将在大规模的数值模拟方面实现高效运行, 从而提升科学研究的效率和产出.

2 分子云化学模型新进展

本节将结合典型分子的研究进展阐述分子云天体化学模型在分子耗尽(如CO、NH₃等)、解吸附过程、含硫分子、复杂有机分子等方面的研究进展以及存在问题 and 未来的研究方向.

2.1 分子的吸附与耗尽

在星际分子云中, 许多分子都存在耗尽的现象, 典型的分子有CO、NH₃和含硫分子等. 耗尽现象描述了高密度分子云中, 分子由于热运动与冷的尘埃颗粒发生碰撞, 其热运动能量低于吸附能时而被吸附在尘埃表面, 并在尘埃上逐渐累积形成冰壳层, 进而导致了在气相观测到的该分子的丰度降低的现象.

以CO为例, 图2展示了在不同源中CO分子的耗尽参数随气体密度的变化, 可见随着密度的增大, 耗尽也不断变大. 从模型与观测的符合度的角度来讲, 单一的模型很难同时对所有的观测数据达到很好的符合, 这也说明人们需要根据特定的源的物理和化学性质, 进行特定的化学建模, 才能达到具体问题具体分析, 深入挖掘源的物理化学性质的目标. 从观测数据的完备性角度来讲, 目前高密度分子云中CO耗尽系数较为缺乏, 这是因为高密度的区域耗尽已经十分严重. 高精度和灵敏度的射电观测将有助于补充缺失的数据, 完善对模型的限制.

氨分子(NH₃)是另外一个重要的分子, 其可作为气

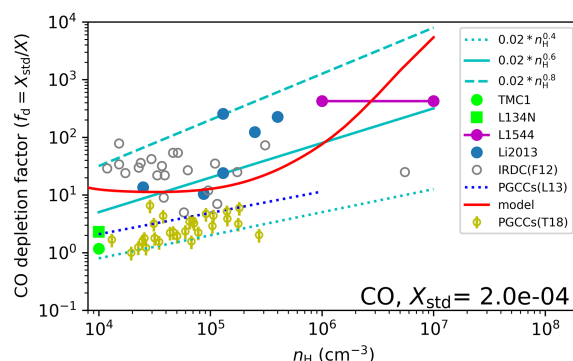


图2 (网络版彩色)冷暗分子云中CO分子的耗尽系数. $f_d = X_{\text{std}}/X$, 是CO丰度与对应气体密度为 10^4 cm^{-3} 时的标准值 $X_{\text{std}} = 2 \times 10^{-4}$ 之比. IRDC: infrared dark clouds (F12^[38]); PGCCs: Planck Galactic Cold Clumps (T18^[39], L13^[40]给出的耗尽系数与气体密度的拟合关系为 $f_d = 0.069 n_H^{0.37}$). 青色线代表文献中给出的与气体密度相关的CO分子耗尽系数形式^[38]. 对L1544^[41](紫色点线), 考虑到L1544的密度不确定性而采用了不同气体密度值. 红色线展示了一个采用了修正的自由塌缩物理模型的天体化学模型的结果($n_H = 3 \times 10^3 \rightarrow 10^7 \text{ cm}^{-3}$). 其他数据来源: TMC-1^[42], L134N^[42]

Figure 2 (Color online) The CO factor in cold dark molecular clouds. $f_d = X_{\text{std}}/X$, is the ratio of CO abundance to the standard value of $X_{\text{std}} = 2 \times 10^{-4}$ at 10^4 cm^{-3} . IRDC: infrared dark clouds (F12^[38]); PGCCs: Planck Galactic Cold Clumps (T18^[39], L13^[40] derived a fitted form as $f_d = 0.069 n_H^{0.37}$. The cyan lines indicate the forms from F12^[38]. For L1544^[41] (purple points), two values of gas density are considered with consideration of the density uncertainty. The red line shows a collapsing astrochemistry model ($n_H = 3 \times 10^3 \rightarrow 10^7 \text{ cm}^{-3}$). Other sources: TMC-1^[42], L134N^[42]

体温度的估算工具. 在冷暗云中, NH₃的丰度量级约为 10^{-8} . 在比较著名的无星核L1544中, NH₃的丰度约为 8×10^{-9} ^[43,44]. 尽管关于NH₃的模型已经考虑了已知的物理和化学机制, 其在L1544中心耗尽的问题并没有得到解决, 即观测上的非耗尽与模型上的耗尽的差异^[45]. 但有直接的观测证据表明, 在原恒星核中NH₃展现出耗尽, 并在气体密度大于 $2 \times 10^5 \text{ cm}^{-3}$ 时以密度的幂律形式($n_H^{-1.1}$)下降^[46], 表明了高分辨率观测的重要性, 也展现出在不同观测源内, 其物理与化学耦合的性质重要性.

中性分子一般都会发生吸附和耗尽的过程, 但由于分子的吸附能各有不同而展现出不同的耗尽现象. 下一节中将讨论解吸附过程的新进展, 并探讨吸附能方面的新研究.

2.2 解吸附过程

与耗尽现象相对应, 解吸附过程同样重要. 在冷暗分子的环境下(10 K), 尘埃冰表面分子的解吸附过程分

机分子,特别是生命前体分子在冷云中丰度较低^[66],信号较弱,因此很难探测到.但随着分子云进一步被原恒星加热形成热分子云核,高温引起的热解吸附过程使得大的分子在气相增丰并得以被观测.作为氨基酸丙氨酸的前体分子的次乙亚胺(CH_3CHNH),其在热分子云核中被探测.它的形成被解释为分子云阶段中尘埃表面的加氢过程($\text{CH}_3\text{CN} \xrightarrow{\text{H}} \text{CH}_3\text{CNH} \xrightarrow{\text{H}} \text{CH}_3\text{CHNH}$)或者是自由基间的反应过程($\text{CH}_3 + \text{H}_2\text{CN} \rightarrow \text{CH}_3\text{CHNH}$),以及可能的气相反应通道($\text{NH} + \text{C}_2\text{H}_5 \rightarrow \text{CH}_3\text{CHNH} + \text{H}$)^[66].关于热分子云核中更加详细的研究,超出本文范畴,不再展开讨论,请阅读相关文献^[67~79].另外,研究表明遥远星系与TMC-1分子云的化学组成相似^[80],因此对TMC-1的持续的分子搜寻,将随着更加先进的仪器和望远镜投入使用而有望得到突破.

2.5 模型与观测符合度

截至目前,已经有超过320个分子在星际空间被观测到(参见CDMS分子列表: <https://cdms.astro.uni-koeln.de/classic/molecules>).此处以典型的冷暗云TMC-1为例,展示目前模型与观测的符合度并探讨未来的发展趋势.在TMC-1中已经观测到超过140多种分子^[42,81~85],其中不乏有机分子、含硫分子和同位素分子等.图4展示了一个典型的天体化学模型($n_{\text{H}} = 10^4 \text{ cm}^{-3}$, $T = 10 \text{ K}$)给出的最佳拟合分子丰度(同位素分子)与观测丰度的比值(仅限于当前模型已有的67个分子^[42,81~84]),可见大部分分子的丰度能够被模型重现在一个量级以内(这与化学模型本身的不确定性分析研究给出的不确定度相当^[86]).但对于一些分子,其符合度稍差,差异甚至可以达到几个量级.可见,模型与观测的整体符合度还有很大的提升空间.

一般来讲,在模型中只关注于几个分子丰度的重现比较容易达到一个量级以内的符合度,但是如果整体考虑一个观测源中所有的分子,其符合度很难有大的提升.这种差异来自多方面,主要有:(1)物理参数的不确定性(如望远镜的波束较大造成了物理参数的不确定性较大.或者,物理模型过于简化,如采用简单的球状模型,而忽略了三维结构的重要性^[37,87,88]等).(2)化学反应参数的不确定性(如化学反应的缺失、吸附能的不确定等).(3)化学模型里的物理和化学机制的不足或缺失(如解吸附机制的不确定等).因此,天体化学模型

的结果与天文观测结果的高度符合,还有很长的路要走.它需要从射电天文观测、化学反应参数、物理和

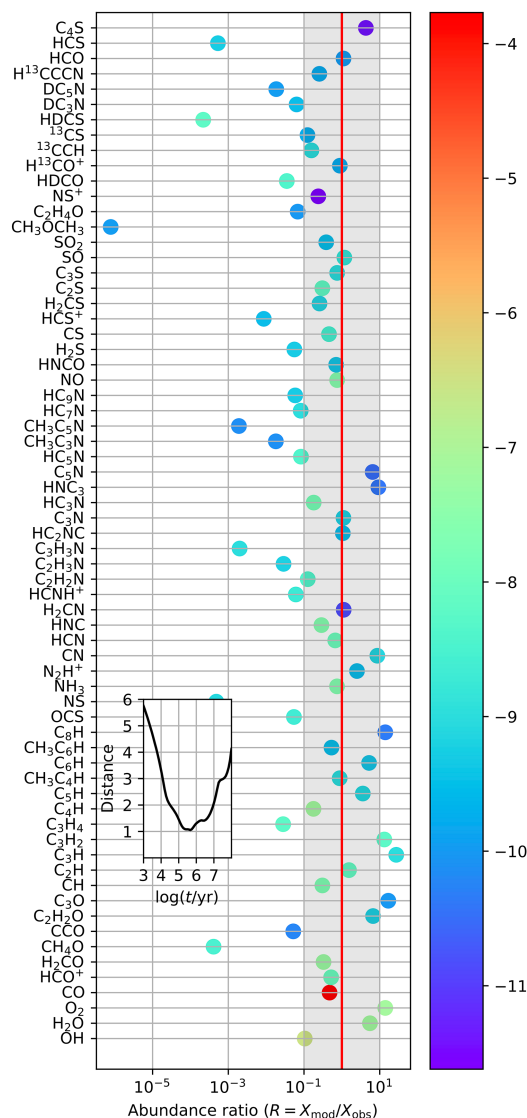


图4 (网络版彩色)TMC-1中观测到的分子丰度与天体化学模型($n_{\text{H}} = 2 \times 10^4 \text{ cm}^{-3}$, $T = 10 \text{ K}$)的最佳拟合丰度的比值.红色线标记比值为1,浅灰色区域标记上下一个量级的范围,点的颜色标记观测丰度的对数值($\log(X_{\text{obs}})$).内嵌图展示观测值与模型值的平均差距($D = [\sum_i^N |\log(X_{\text{obs},i}) - \log(X_{\text{mod},i})|]/N$),最佳拟合年龄为 5×10^5 年.注意: ^{13}CCH 和 HDCS 观测丰度为上限^[81]

Figure 4 (Color online) The abundance ratios of species between the observed values of TMC-1 and the best fitted values of the astrochemistry model ($n_{\text{H}} = 2 \times 10^4 \text{ cm}^{-3}$, $T = 10 \text{ K}$). The red line indicates value of 1.0 and the light gray region indicates one order of magnitude around 1.0. The colors of the points represent the logarithmic values of the observed abundances. The in-set panel shows the overall average value of distance between observation and model ($D = [\sum_i^N |\log(X_{\text{obs},i}) - \log(X_{\text{mod},i})|]/N$). The best fitted age is 5×10^5 years. Note: the values for ^{13}CCH and HDCS are upper limits^[81]

化学建模等多个方面持续提高精度和完善数据,才能有所发展和突破。

2.6 机器学习

随着天文海量数据的不断积累以及数据精度的要求越来越高,即便是使用速率方程的化学模型,也在面对大规模密集计算时显得十分耗时,特别是当考虑天体的物理和化学性质(例如:辐射转移、三维结构以及磁流体动力学过程等)越来越复杂时,耦合后所需的计算资源是巨大的。随着计算机技术和算法不断提升,机器学习的方法得以快速地发展。基于海量天文数据的天体化学模型方面的机器学习在最近几年更是发展迅速。

基于速率方程的单点天体化学模型,可以根据给定的目标点的物理性质和化学反应网络,快速给出随时间演化的分子丰度信息。但对于真实的星际分子云环境,其每一个空间点都有不同的物理和化学性质,且处在某一独特的演化阶段。因此,大规模的多点计算是获得接近于真实值的必要条件。这一过程的缺点是将耗费大量的计算资源。通过构建大规模的多点模型,耦合多样的物理条件和化学参数,即可通过机器学习的方法加以训练来建立物理条件与化学结果之间的联系,即为机器学习在天体化学模型方面的直接应用^[89-91]。这样,基于机器学习的训练结果,给定物理条件,就可以快速地给出最可能接近真实的结果,大大缩短了计算时间。进一步地,将分子丰度与辐射转移相结合进行

数值计算,在分子谱线物理性质的预测方面也大大提升了效率和可靠性^[92]。同时,基于神经网络的算法,也在天体化学模型方面得以发展,展现出了很好的执行效率(效率提升1000倍以上)^[93-95]。随着天文海量数据的不断积累、机器学习等算法在天体化学模型方面不断的深度应用,天体化学模型将会对星际分子云的空间、物理和化学信息给出更真实、精确和详尽的刻画。

3 总结和展望

天体化学模型作为星际空间中分子相关的物理和化学过程研究的不可或缺的重要工具,为人们理解和验证极端天文环境下的化学过程提供了关键信息和帮助。从简单的纯气相天体化学模型,发展到考虑尘埃颗粒表面的两相模型,再发展到考虑尘埃冰壳层的三相模型,天体化学模型在近30年来得到了快速的发展。实验室数据的不断累积、数值计算技术的不断发展和成熟、新的测量参数和物理化学机制不断发现,使得与天文观测的符合度不断提高。伴随着近几年来的人工智能技术的发展,天体化学也在此方面展现出了蓬勃的活力。

本文结合典型分子云讨论了上述有关天体化学模型发展的几个方面,并对其中存在的问题进行了探讨,希望能起到抛砖引玉的目的,为天体化学模型方面的研究提供新的视角和思路。

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Summary for “分子云天体化学模型的进展”

The advancements of astrochemistry models of molecular clouds

Ji-Xing Ge^{1,2*}, Wen-Zhong Cai^{4,5,1}, Xia Zhang^{1,2,3}, Fang-Fang Li^{1,2} & Jing-Jing Wang⁵

¹ Xinjiang Astronomical Observatory, Chinese Academy of Sciences, Urumqi 830011, China

² Xinjiang Key Laboratory of Radio Astrophysics, Urumqi 830011, China

³ Key Laboratory of Radio Astronomy and Technology, Chinese Academy of Sciences, Beijing 100101, China

⁴ College of Science, China University of Petroleum-Beijing, Beijing 102200, China

⁵ Faculty of Science and Arts, China University of Petroleum-Beijing at Karamay, Karamay 834000, China

* Corresponding author, E-mail: gejixing@xao.ac.cn

Molecular cloud is the key initial stage of star formation. With the physical conditions which is suitable for formation of various molecules, the molecular clouds become the targets to be studied using radio telescopes by astronomers. To know the chemical processes of molecules in space, astrochemical studies started a few decades ago. Astrochemistry is an interdisciplinary frontier discipline that merges astronomy, physics, and chemistry, integrating astronomical observations, laboratory chemistry, and numerical simulations. Over the past few decades, it has yielded rich results. Astrochemical models, as a primary aspect, play a crucial role in understanding the physical and chemical formation mechanisms of molecules in interstellar molecular clouds. By simulating the details of chemistry in both gas-phase and solid-phase on the cold dust grains, it provides more and more information of physical and chemical properties/processes in molecular clouds at different evolutionary stages. This review introduces the development of astrochemical models, numerical simulation methods and procedures, with a focus on the latest advancements in physical and chemical mechanisms. This paper covers the fundamental aspects of numerical methods in astrochemical models, including databases and numerical simulation programs. A brief introduction of the rate equation methods and Monte Carlo numerical methods is given to highlight the basics. Using astronomical observational data and typical representative molecules such as CO, NH₃, OCS, and organic molecules, the paper elaborates on the achievements and shortcomings of astrochemical models in molecular adsorption and desorption, the main molecular forms of sulfur and the composition of ice on dust grains, as well as the formation of complex organic molecules in the ice. In molecular clouds, more than 320 species have been detected which hints abundant chemistry. Taking the rich molecular abundance observations in the typical molecular cloud of TMC-1 as a sample with more than 140 species observed, this paper compares the molecular abundances with the results of astrochemical models that include isotopologues, showing the agreement between the astrochemical models and observations, and discussing the discrepancies and the future needed improvement between observations and models. The fitting result indicates that the overall agreement for 67 species, encompassing simple molecules, complex organic species, and isotopes, is insufficient to attain an agreement within one order of magnitude. This means that the improvement of the model is highly required. Finally, this paper discusses the development and application of machine learning in astrochemical models. With the continuous upgrading of astronomical observation technology and equipment, the updating of models and numerical calculation algorithms, as well as the improvement of laboratory measurement data, the research on astrochemical models of molecular clouds will have a significant development.

astrochemistry, molecular clouds, molecular abundance, numerical simulation

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