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新型污染物大区域污染扩散及其浓度预测的研究：从机理模型到智能算法

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摘　要

新型污染物(如多环芳烃)因其持久性和潜在健康风险，已经成为当前研究的热点。在区域乃至全球尺度上准确模拟其扩散行为与预测浓度变化，对于制定污染防控政策和开展健康风险评估具有重要意义。本文系统回顾了新型污染物在大气中扩散和迁移的基本理论基础，梳理了当前统计模型和机器学习以及深度学习预测模型的适用场景，重点分析了不同模型在处理复杂污染过程的表现差异，探讨了多种暴露–反应模型(如分布式滞后非线性模型)在污染物浓度与呼吸系统、心血管系统疾病以及慢性阻塞性肺疾病(COPD)发病率和死亡率分析中的应用现状与挑战。研究指出，个体暴露估计不确定性、区域差异性及多污染物交互作用仍是当前健康风险评估的难点。未来，构建多源数据驱动的高分辨率预测体系，建立污染物浓度–健康影响的一体化模型方法，将是提高大气污染治理效能的关键方向。

关键词

新型污染物，统计模型，深度学习，健康暴露

Regional-Scale Dispersion and Concentration Prediction of Emerging Pollutants: From Mechanistic Models to Intelligent Algorithms

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Abstract

Emerging pollutants, such as polycyclic aromatic hydrocarbons (PAHs), have been identified as a focal point of current research due to their persistence in the environment and potential health risks. Accurate simulation of their atmospheric dispersion and concentration dynamics on regional and global scales is considered essential for the formulation of pollution control policies and the conduction of health risk assessments. In this review, the fundamental theoretical basis of pollutant dispersion and transport in the atmosphere is systematically outlined, and the applicable scenarios of current statistical models, machine learning, and deep learning-based prediction approaches are examined. Particular emphasis is placed on the performance differences of various models in addressing complex pollution processes. Additionally, the application status and challenges of multiple exposure-response models (e.g., Distributed Lag Non-linear Models, DLNMs) are discussed with regard to their use in analyzing associations between pollutant concentrations and respiratory diseases, cardiovascular diseases, and chronic obstructive pulmonary disease (COPD) incidence and mortality. Persistent challenges such as uncertainties in individual-level exposure estimation, regional heterogeneity, and multi-pollutant interactions are highlighted in current health risk evaluations. Looking forward, the development of high-resolution, multi-source data-driven prediction frameworks and the establishment of integrated models linking pollutant concentrations with health outcomes are expected to be key in enhancing the effectiveness of air pollution control strategies.

Keywords

Emerging Pollutants, Statistical Models, Deep Learning, Health Exposure

1. 绪论

新型污染物是指近年来被广泛关注但没有被纳入传统监管体系的一类环境污染物，具有持久性、生物积累性和潜在毒性等特点[1]-[3]，以多环芳烃(PAHs)为代表的新型有机污染物[4] [5]，来源广泛，包括燃煤、汽车尾气等，由于气候变暖，部分水体形成二次污染源，在环境中通过气－粒转化，沉降再挥发等机制形成多介质迁移。除 PAHs 外，新型污染物还包括全氟、多氟化合物[6] [7] (PFAS)、药物与个人护理品[8] [9] (PPCPs)、内分泌干扰物[10] [11] (EDCs)等，对于新型污染物环境行为的研究逐步成为全球环境治理和风险评估的重点。多环芳烃(PAHs)是一类具有高稳定性和疏水性的有机污染物[12] [13]，广泛存在于我们周围的环境中，比如空气、水体、土壤，甚至食物中都可能检出[14] [15]。随着工业化和城市化的发展，人类活动越来越频繁，PAHs 的来源也变得更加复杂。过去，这类污染物主要来自煤炭、木材等含碳材料燃烧不完全时产生的烟气。但现在，像机动车尾气、工厂废气、餐饮油烟、垃圾焚烧以及石油化工过程等[16]，也都成为了重要的排放源，使得 PAHs 在环境中无处不在。

在这类污染物中，菲(Phenanthrene，简称 PHE)是一个比较有代表性的“成员”。它属于低分子量的三环 PAHs，常常在空气、水、土壤、沉积物这些环境介质中都能被检测到[17]。相比一些结构更复杂的 PAHs，PHE 的分子结构更简单、性质也比较稳定[18]，而且检测技术已经很成熟，因此它更容易被监测和研究。此外，因为 PHE 的迁移、降解等环境行为跟其他低分子量 PAHs 很相似，科学家们常常把它当

作一种“指示物”，通过研究它来了解这一类污染物在环境中的表现和趋势。随着人类活动的不断加强，PAHs 在环境中的浓度越来越高，分布也变得更加复杂。这些污染物不仅在空气、水体和土壤等不同介质之间不断迁移和累积，导致更容易接触到它们，健康风险也随之增加。研究发现，PAHs 可以通过吸入空气、摄入被污染的食物，甚至皮肤接触进入人体[19]，在体内逐渐积累，可能引起包括 DNA 损伤[20]、基因突变[21]、免疫系统紊乱和内分泌干扰[22]等多种健康问题。其中一些高毒性的 PAHs 甚至已经被世界卫生组织下属的国际癌症研究机构(IARC)列为可能或确定对人类有致癌性的物质[14]。虽然 PHE 的毒性比那些高分子量的 PAHs(如苯并[a]芘，Benzo[a]pyrene)相对弱一些，但它仍然有一定的毒性，尤其是在长期接触的情况下，仍可能对健康造成不良影响。儿童、孕妇等敏感人群更容易受到伤害[23]。因此，PHE 常被用在环境监测和模拟研究中，不仅可以帮助评估污染水平和潜在健康风险，也能用来观察这类污染物在自然环境中的迁移路径和最终去向。

2. 全球与区域尺度大气污染模拟方法

2.1. 模拟的基本原理与理论基础

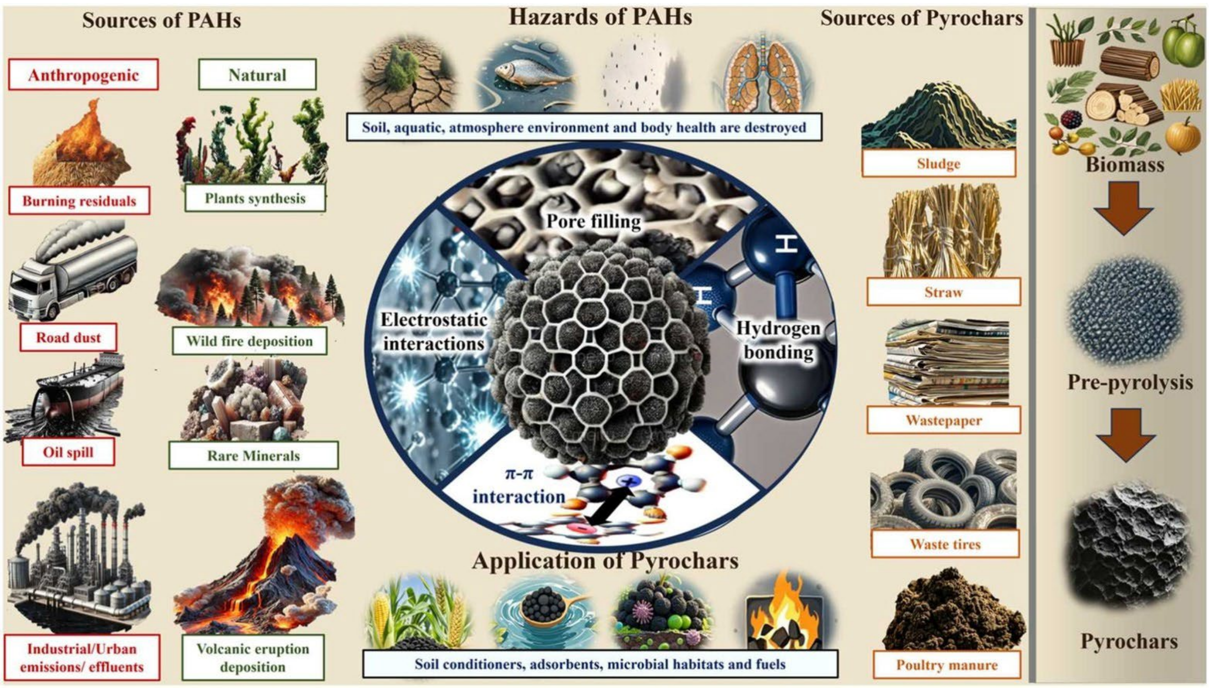

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Figure 1. Sources and hazards of PAHs [24]
图 1. PAHs 的来源及危害[24]

多环芳烃(PAHs)是生态系统面临的长期遗留的环境问题，图 1 是 PAHs 的来源和危害。由于全球气候变暖导致部分次要污染源的产生，这意味着 PAHs 会产生二次排放[25] [26]。在大气传输过程中，大多数空气污染物，如 PAHs，通常集中分布在地表上空 1 公里以内的大气边界层中[27]。并且，在夜间，由于地面冷却，大气变得稳定，形成一个浅而稳定的夜间边界层[28]，高架源(比如高烟囱)排放的污染物在夜间无法向下扩散到地表[29]，于是它们往往停留在边界层顶部或在边界层之上，白天太阳升起后，地面开始加热，形成热对流和湍流[30]，边界层逐渐发展并升高。这个过程中，夜间滞留在边界层顶部或上方的污染物随边界层的上升被“卷”入混合层，向下传输到地面，污染就出现在地面空气中，这一过程叫

向下混合[31]。大气污染物的转化是指污染物在大气中经历的一系列化学变化过程。在大气环境中，许多化合物通常会被氧化，进而发生转化。这些转化反应主要包括光化学反应和热反应[32]。其中，光化学反应是指化学物质在阳光中受到光子激发后发生的反应，通常会生成具有较强反应活性的中间产物。这些中间产物随后可能继续发生一系列热反应，即在无光条件下通过热力学途径发生的化学转化，从而生成新的污染物或衍生物。多环芳烃(PAHs)在大气中经历复杂的气相化学反应和气溶胶动力学过程。以菲(PHE)为代表的低分子量 PAHs 主要以气态存在，能与羟基自由基、臭氧和硝酸根自由基等发生反应，生成氧化或硝化产物，如羟基菲或硝基菲，部分产物具有更高毒性[33]。同时，受温度和颗粒物特性影响。当菲吸附于气溶胶表面后，还可发生异相氧化反应，并通过干沉降、湿沉降和气体沉降从大气中去除，干沉降[34]是从大气中去除污染物的重要机制，干沉降涉及一系列物理和化学过程，与自然或人造表面接触，粘附或溶解在这些表面上，从而从大气中去除。湿沉降[35]是通过沉淀沉积大气中的物质的过程，涉及如钙离子,它们通过影响养分循环和维持土壤和水中的酸碱平衡，在影响生态系统健康方面发挥重要作用。气体沉降是指 PAHs 在土壤中和空气中的持续迁移和平衡，称为土壤－空气交换[36]。

PHE 作为一种典型的多环芳烃，在大气中主要以气相和颗粒相存在，通过化石燃料燃烧、垃圾焚烧和森林火灾等排放到大气中，它在大气中部分以气态存在，部分吸附在颗粒物上，PHE 在大气传输分为水平传输和垂直传输两个过程[37]、在水平传输的过程中，气相 PHE 可以通过大气环流跨区域传输，进行远距离传输[38]，而颗粒相 PHE 随颗粒物进行中等距离传输，但由于重力沉降和干湿沉降，传输距离有限。在垂直传输的过程中，PHE 可以在边界层内上下混合，在不稳定的大气条件下，PHE 容易向上扩散至高空，有助于远距离传输。PHE 的大气降解过程主要经历气相反应和颗粒相氧化两类过程[39]。PHE 的干沉降包括粒子吸附的 PHE 直接沉降到地面、水体、土壤中，湿沉降通过雨雪来洗涤大气中的气相和颗粒相 PHE。自然过程主要通过干沉降和湿沉降两种途径来去除大气中的 PHE[40]，但沉降过程不排除形成二次污染源的问题，因此有效去除大气中的 PHE 仍是人类面临的一个严峻课题。

2.2. 模型类型与分类

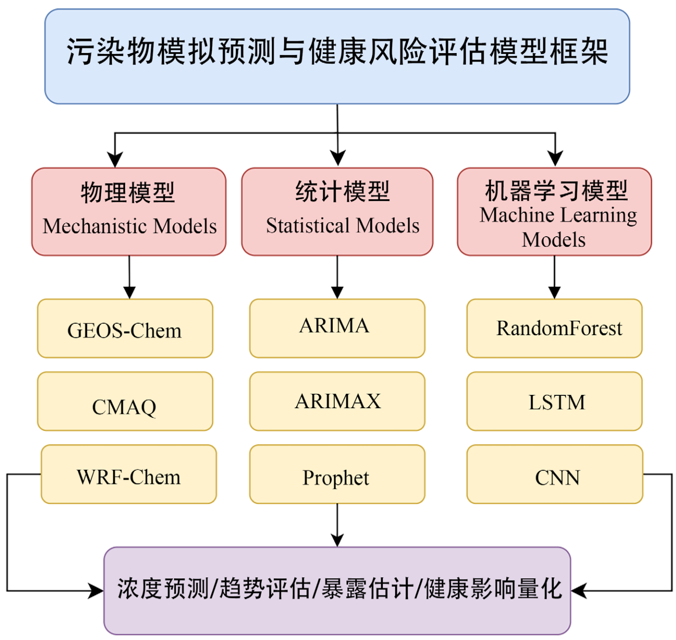

Figure 2. Pollutant simulation prediction framework diagram
图 2. 污染物模拟预测框架图

污染物模拟预测框架图如图 2 所示，天气研究预测与化学耦合模型(WRF-Chem) [41]被广泛应用于空气污染物的预测与模拟。空气污染的形成与演变涉及多种气象因素，如风速和风向、湍流、太阳辐射、云和降水等，同时还包括复杂的化学过程，如污染物的转化、沉积以及与气溶胶之间的相互作用。WRF-Chem 模型[42]的一个显著特点是化学与物理过程的高度耦合：化学成分不仅受气象条件驱动进行传输和扩散，同时也会通过辐射与气溶胶相互作用反过来影响大气动力学过程，如气温、云形成等。这种双向耦合机制使得 WRF-Chem [43] [44]在模拟空气质量和研究大气化学与气象之间的相互关系时具备更高的物理真实性。在此基础上，美国国家大气研究中心(NCAR)的大气化学观测与建模(ACOM)实验室正与全球大气化学研究社区合作，开发一种新一代的大气化学建模框架——(Multi-Scale Infrastructure for Chemistry and Aerosols, MUSICA)建模系统[45] [46]，该模型基于多尺度化学和气溶胶模拟原理，能够从全球尺度模拟大气环流和污染物长距离传输，同时解析更细尺度上的排放、化学转化及人类暴露过程。这一框架旨在实现从局地到全球的统一建模。美国国家空气质量预报能力(National Air Quality Forecast Capability，NAQFC) [47]是由美国国家海洋和大气管理局(NOAA)与美国环境保护署(EPA)联合开发的国家级空气质量预报系统。该系统核心采用了 EPA 的社区多尺度空气质量模型(CMAQ) [48] [49]，这是一个集成了气象、排放、化学输送与污染物沉降等模块的三维化学输送模型，具备较强的污染物输送、转化和浓度变化模拟能力。NAQFC 通过将气象预测模型与 CMAQ 模型耦合，实现了对美国全国范围内 O_3、PM_{10}、$PM_{2.5}$ 等污染物的实时预测与 48 小时逐小时预报。CHIMERE 模型是欧洲广泛使用的大气化学输送模型之一，基于 CHIMERE [50]提供全国范围内的高分辨率空气质量分析、预报与公共预警服务。CHIMERE 模型支持每日更新的实时模拟，结合观测数据进行同化，提高预报准确性。其模拟能力涵盖从区域到城市尺度，具备灵活的化学机制设置、详细的颗粒物和气体物种处理模块，并能耦合多种排放源与气象数据，是开展空气污染评估、政策制定和健康风险研究的有力技术支撑。

GEOS-Chem 是一个全球性的三维大气化学输送模型[51] [52]，由美国国家航空航天局(NASA)全球建模与同化办公室(GMAO)开发并持续支持。GEOS-Chem [53]-[56]广泛应用于全球和区域尺度的大气成分模拟研究，是当前国际上最具影响力和广泛应用的大气化学模型之一。GEOS-Chem 支持区域嵌套模拟，目前已实现包括东亚、北美、欧洲和中东等多个区域的高分辨率建模，空间分辨率最高可达 0.2500° × 0.3125°，适用于研究局地污染过程与全球背景浓度的相互作用。该模型采用模块化架构与高度并行化设计，支持 OpenMP 和 MPI 并行计算框架，具备良好的扩展性与计算效率，可适配多种高性能计算环境。自版本 13 后，GEOS-Chem [57]进一步实现与地球系统模型对接的能力，成为开展多尺度、大气成分—气候耦合模拟的重要平台。使用 GEOS-Chem 模型进行全球尺度的污染物模拟，能够实现高空间和时间分辨率的模拟效果，适用于对污染物的长期时间和空间变化趋势进行深入研究，GEOS-Chem 基于最新的气象数据和排放清单，能够对如臭氧，VOCs 和 PAHs 等进行深入的浓度模拟和研究分析。GEOS-Chem [58]-[60]模型在模拟大气 CO 和 CO_2 的浓度方面表现良好，能够在经纬度分布以及高度上进行较为准确的模拟，通过对地面观测数据和卫星反演数据的对比。此外，GEOS-Chem 模型具有高度模块化的结构，例如在 HEMCO 模快引入了较为完整的排放清单，MAPL 模块[61]专门用于地球系统系统建模的中间层库，由 NASA GMAO 开发，用于简化(Earth System Modeling Framework, ESMF)的使用，KPP 模块可以自动生成化学反应速率代码，支持用户自定义化学反应，并且还有适合多种分类污染物模拟的模块，如 fulchem 模块、POPs、Carbon 等模块，并且 GEOS-Chem 的耦合性强，可以接入其他地球模拟系统或者数据平台，如 WRF-GC 系统[62]，在 WRF-GC 模型中，气象场与化学过程被统一地计算在完全一致的三维网格系统上。为确保质量守恒和数值一致性，模型采用相同的对流输运方案和时间步长对气象变量和化学物种进行处理，从而实现两者在空间和时间上的高度耦合与协调。

哈佛大学的工程与应用科学学院(SEAS) [63]研究团队在最新研究中将 GEOS-Chem 大气化学模块成

功集成到 CESM2 (Community Earth System Model version 2)中，替代原有的 CAM-chem 模块，这一集成体现了模型模块化可移植的优势，同时也增强了 CEMS2 模拟对流层化学过程的能力，研究团队进一步通过多源观测数据如臭氧探空、地面观测站、ATom-1 等对模型模拟结果进行评估，对比结果得出，GEOS-Chem 在 CESM2 框架中对对流层的研究具有较高的准确性，能够进行高质量的模拟，同时具备为其他大气化学研究方法提供模块化替代方案的潜力。南京信息工程大学的研究团队[64]通过将 GEOS-Chem 全球化学输送模型与高级粒子微物理模型(APM)耦合，深入研究粒子数浓度和新粒子的形成过程，为区域新粒子生成研究提供了模型支持和验证依据。这一工作显著提升了对大气颗粒物形成机制的理解，有助于改进空气质量预测研究。南方科技大学的研究团队发布了 WRF-GC v2.0 模型[65]，实现了区域气象模式 WRF 与全球大气化学模式 GEOS-Chem 的双向在线耦合，支持气溶胶对辐射和云微物理过程的反馈，并具备嵌套域和高性能并行计算能力。研究还通过模拟实验验证了模型在再现 $PM_{2.5}$、臭氧及多种气象变量空间分布方面的准确性。

GEOS-Chem 作为一个全球三维化学传输模型涵盖大气化学、气溶胶物理、排放和沉降多种过程，在研究大气成分的时空分布和演变具有显著优势。在大气污染、臭氧层变化、气溶胶影响、健康风险评估等领域具有广泛应用。

2.3. 统计方法预测污染物浓度

自回归积分滑动平均(AutoRegressive Integrated Moving Average, ARIMA) [66]模型是一种经典的时间序列预测模型，它是一种经典的线性时间序列建模方法，在污染物的预测中，ARIMA 适用于没有复杂外部影响因素，但存在一些较为显著的趋势或者周期性变化的污染物浓度预测，通过将自回归(AR)、差分(I)和滑动平均(MA)三个部分结合，用于建模和预测单变量。研究[67]聚焦于印度新德里部分污染严重但数据稀缺的城市，采用 ARIMA 模型 $PM_{2.5}$ 浓度进行预测。结果显示 ARIMA 模型在该地区具有较好的预测性能，RMSE 和 MAE 均表现出较高的准确性，但是该模型依赖于历史数据，无法捕捉外部环境变化对污染趋势的影响，勋在局限，该模型的预测结果具有一定的参考价。SARIMA(Seasonal ARIMA)模型是在 ARIMA 的基础上，增加了对季节性的建模能力，它适用于时间变化中既存在趋势变化和季节性周期波动的污染物浓度预测。研究[68]预测全球 N_2O 排放方面的表现在对比了 SARIMA 和其他两种机器学习模型，三种模型中 SARIMA 的表现最好，误差最小。SARIMA 在特定的污染物浓度预测方面效果不差于机器学习方法，ARIMAX (Autoregressive Integrated Moving Average with Exogenous Variables) [69]是将外部变量引入 ARIMA 框架中，结合了时间序列建模和回归分析的优势。在空气污染研究中，常将气象因素如温度、湿度、风速、降水、气压等引入模型，从而达到更精确的模拟污染物的扩散和沉降的过程。研究[70]探讨了环境因素对流感发病率的影响，并应用 ARIMAX 模型提升预测精度。研究表明，将环境指标作为外生变量引入时间序列模型，有助于更准确地预测流感流行趋势，Prophet 是由 Facebook (现 Meta)于 2017 年开源推出的时间序列预测模型[71]，该模型可以做到在不需要深入统计背景的情况下，提供强大、直观的预测工具，尤其适用于具有明显季节性、趋势性和节假日效应的时间序列数据。基于 Prophet 模型的优势，目前有很多研究团队选择用该模型进行预测研究。传统的线性时间序列方法不足以模拟污染物浓度，而 Prophet 采用广义加法模型来拟合预测函数[72]，Prophet 拟合的速度十分迅捷，能够使用户快递的响应探索模型的不足。利用 Prophet 在非线性、季节性和假期影响建模方面的有效性，提高了预测的准确度。如研究[73]使用 Prophet 模型量化周期性和固定假日对英国水平的影响，展示了特殊节假日如圣诞节，对当地空气的污染。

2.4. 不同机器学习方法预测污染物浓度

传统的机器学习如决策树，随机森林(RF)，支持向量回归被广泛应用于污染物浓度预测，这些方法能

够有效处理非线性关系和多变量输入。研究[74]探讨了四种机器学习算法(随机森林、决策树回归、线性回归和支持向量回归)进行建模，这些传统机器学习方法虽然能够在一定程度上有效处理污染物浓度的变化问题，但是由于它们时序建模和空间相关性有限以及模型的自适应性差，独立分布等缺点[75]。深度学习在污染物浓度预测中展现出非常强的时序建模能力和非线性拟合能力。长短时神经网络(LSTM)在污染物浓度预测具有较好的表现力，特别是最近的深度学习研究中，将 LSTM 和其他模型相结合，具有更好的预测表现力[76]。并有研究[77]提出一种新颖的混合深度学习模型 STL-CNN-BILSTM-AM，用于对 $PM_{2.5}$ 的精准预测。双向 LSTM 也可以结合无监督聚类，用于美国 $PM_{2.5}$ 和臭氧预报偏差矫正[78]，在极端事件预测上具有更好的预测精度。

北京邮电大学的研究团队[79]提出了一种混合预测框架 GC-LSTM，用于在小时尺度上精准预测区域地面二氧化氮(NO_2)浓度。该方法结合了 gcForest 的空间特征学习能力与 LSTM 网络的时间序列建模优势。中南大学研究团队[80]提出了一种基于多子系统协同的双向长短期记忆网络(Bi-LSTM)自适应软传感器，用于实现污水处理过程中氨氮浓度的全局预测。

在污染物浓度预测的研究中，统计方法与深度机器学习方法各有优势和适用的场景，传统统计方法如 ARIMA、ARIMAX、线性回归等具有良好的可解释性[81]，但在处理非线性关系与高维特征方面能力有限。传统机器学习方法如随机森林、支持向量回归、决策树等能较好处理多变量之间的非线性关系，在中小规模数据中较为适用，但缺乏时空建模能力。而近些年兴起的深度学习方法如 LSTM、CNN 和 GCN 等，能够较好的提取时序关系和特征变量，表现出更优的预测精度。在处理复杂污染物浓度预测问题事，采用混合模型处理问题能够进一步提升预测性能。不同模型的特点如表 1。

Table 1. Comparison of the characteristics of different models or methods
表 1. 不同模型或方法的特点对比

模型类型	代表模型/方法	物理/化学机制完备性	计算资源需求	时空尺度适用性
物理模型	GEOS-Chem, WRF-Chem	完整的化学反应和气象机制	非常高	全球区域
统计模型	ARIMA, ARIMAX, Prophet	无物理机制	低	区域尺度
机器学习	RF, LSTM	无物理机制	较高	适应多时空尺度

3. 污染物浓度与健康影响关系

随着全球科技的发展，污染物的种也呈现的多种多样，而它们对于人体健康的威胁是不可忽视的。长期暴露于部分污染物中，可能会对人体带来不可逆转的危害。有研究发现 $PM_{2.5}$ 和老年人慢性阻塞性肺疾病(COPD)密切相关[82]，并且有众多因素如气候、野火等通过影响 $PM_{2.5}$ 水平来影响人体健康[83]。此外，有研究[84]对重庆市城乡地区的 $PM_{2.5}$ 和 PM_{10} 暴露对慢性阻塞性疾病(COPD)死亡率的滞后效应差异进行研究采用分布式滞后性非线性模型(DLNMs)，研究结果表明污染物浓度升高显著增加了 COPD 的死亡风险，并且呈现出一定的空间不平等性。并且有研究[85]基于 2014~2019 年中国某城市的慢性阻塞性肺疾病(COPD)住院数据采用广义加法模型和分布式滞后模型分析了空气污染(如 $PM_{2.5}$、PM_{10})对 COPD 急性发作的影响，研究表明短期户外空气污染暴露可能诱发或加重 COPD。有最新研究[86]表明，有机污染物在炎症性肠病(IBD)中起着一定的依赖作用。该研究对 IBD 患病率和环境污染数据使用图神经网络进行时空依赖关系建模，虽然不同的研究区域有不同的风险差异，但是有机污染物浓度在一定程度上导致了炎症性肠病(IBD)的发生。并且最新研究显示，长期共同暴露于多种环境空气污染物和常见年龄相关的眼病发病率有关[87]，该研究基于英国生物样本库，研究了约 44 万名无眼病人群，构建空气污染风险模型，结果发现长期暴露于多种空低浓度气污染物与三种眼病呈现显著正相关。并且，环境空气污染物与

呼吸和心血管疾病存在一定的相关性。

污染物暴露与疾病负担的研究有助于我们加大针对随环境污染物的防治力度，从而降低疾病的发生，有很多模型可以用来研究污染物和疾病之间的关联性，如分布式之后非线性模型(Distributed Lag Non-linear Model, DLNM) [88]，该模型可以非常好的处理时间序列，能同时建模滞后效应和非线性关系，并且能够有效评估污染物暴露多个滞后日对健康(如死亡率)的影响，还能够建模浓度与风险之间的非线性剂量反应关系。广义线性模型(Generalized Linear Model, GLM) [89]能够比较好的处理线性关系，常用于分析死亡人数和污染物浓度之间的联系。可以使用 Poisson 回归和 quasi-Poisson 方法[90]，可以加入气象向量等控制多种因素变量，但是改模型不能非常好的处理非线性关系和复杂滞后项，广义加性模型(Generalized Additive Model, GAM) [91]考虑到非线性趋势和周期，能够用平滑函数控制季节性和长期趋势。

4. 总结

环境治理是一个全球性的课题，尤其在当前全球气候变化、城市化快速发展的背景下。在模型构建方面，首先要明确污染物模拟的基本理论，如扩散、对流、化学转化的过程，分析不同模型的特征和应用场景，识别污染物的变化规律，通过精细的化学机制模块，能够对污染物的生成、迁移与转化过程进行动态模拟，适用于区域和全球尺度的污染源模拟。在污染物预测方法上，预测作为辅助甚至替代模拟的一种手段，近年来得到迅速发展。针对不同地区尺度、时段周期、污染物种类，统计方法和机器学习方法各有优势，如 ARIMA 等统计方法具有良好的可解释性，适合周期比较短、线性趋势比较明显的模拟，而机器学习方法如随机森林和深度学习方法如 LSTM 在处理高纬度、非线性并且比较复杂的污染预测任务时呈现较高的精度，将多种方法集成起来形成混合模型是污染物浓度研究的一个趋势，有助于提升模型的准确性和稳定性。在健康风险评估方面，DLNM 等方法被广泛应用于研究污染物浓度和疾病或人口死亡率的关系。针对一体化模型，可将大气污染物的传输扩散方程嵌入深度学习框架，构建具备物理约束的神经网络模型(如 PINN)。该模型兼顾数据驱动的预测能力与物理机制的一致性，有助于提高污染浓度模拟的精度与可解释性。

5. 挑战与局限性

污染物模拟与预测高度依赖高质量、多源异构的数据，然而在实际中，观测数据的空间覆盖不均匀、排放清单存在不确定性、气象驱动数据分辨率有限，均会影响模型性能。现有模型在物理机制完整性与数据驱动能力之间难以取得平衡。传统物理模型计算资源消耗大、参数复杂，适用性受限，而数据驱动模型虽能高效建模复杂非线性过程，却易受数据质量制约，且普遍存在可解释性不足的问题。此外，不同研究方法之间缺乏统一的评价体系，模型泛化能力差，不利于跨区域、跨污染物的推广应用。在复杂环境背景下，模型对极端污染事件的响应能力亦存在明显不足。为推动相关研究向更高精度、更强鲁棒性方向发展，更需在数据融合、物理模型嵌入、机器学习与不确定性量化等方面开展深入探索与交叉创新。

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