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Identifying air pollution characteristics, source apportionment methods, and air quality modeling approaches in transport hub settings: State-of-play and future directions

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ABSTRACT

This review synthesises the current state-of-the-art in air quality (AQ) research relating to current monitoring and modeling methods focused on transport hub (TH) settings. Air pollution characteristics from monitoring studies revealed that higher concentrations of $PM_{2.5}$ (12.4–147.8 μg/m^3) and SO_2 (54.1–78.3 μg/m^3) dominated AQ issues in ports. Train terminals were impacted by NO_2 (52.2–472.5 μg/m^3), with VOCs (123–973 ppb) and UFPs (5×10^3 to 4.8×10^6 particles/cm^3) considerably higher at airports. Bivariate polar plots, data filtration techniques, and regression models were considered relatively simple, resource-efficient, and effective source apportionment methods to assess AQ (SO_2, NO_2 and UFP) from sources in and around THs. Speciated receptor modelling was more expensive, but is suitable for complex environments to evaluate multi-pollutant (PM and VOCs) conditions. Gaussian models demonstrated better agreement than Eulerian and Lagrangian models at airports, with Eulerian models slightly outperforming Gaussian models in port settings. Additionally, Eulerian was the most effective methods to model secondary pollutants and over long distances. Limited AQ research focused on small-scale semi-enclosed THs, such as bus and train terminals, with an additional knowledge gap of indoor AQ in port and airport buildings. Improved characterisation of pollutants like VOCs, BC, and PAHs would benefit climate and health impact assessments at THs, with the integration of AI offering a means to enhance monitoring and management AQ at Tin these settings in the future.

1. Introduction

Air pollution is a global challenge that has significant economic and health impacts (Manisalidis et al., 2020; Sivarethinamohan et al., 2020). There is considerable evidence on the wide range of health effects associated with air pollution, which include premature mortality, impaired fertility outcomes, lower birth weight, cardiovascular and respiratory diseases, lung cancer and strokes (Chawala et al., 2023; Priyan et al., 2023; Shanmuga et al., 2021). As 4.2 million premature death were associated with outdoor air pollution exposure worldwide in 2019 (WHO, 2022), and as approximately 99 % of the global population live in areas with air pollution levels that exceed WHO guidelines (WHO, 2022) it is not surprising that air pollution exposure accounts for >11 % of all premature deaths globally (Landrigan et al., 2022). Despite strong efforts to decrease emissions through diverse means, air pollution from the transport sector persists to be a main source of elevated concentrations of air pollution in the urban environment today (Zhu et al., 2021). While attention has been mostly paid to the automotive industry, concerns have also been raised about the impact of emissions from various TH such as airport, port, bus, and train terminals on its surrounding environment (de Mendonça Ochs et al., 2015; Font et al., 2020; Xu et al., 2023; Zhang et al., 2019). While a TH facilitates mass movement of people and goods, it can also be responsible for high quantities of air pollution. Although, travellers only spend a limited time at a THs (especially, train and bus terminals) exposure to high pollutant

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Abbreviations

ADMS	Atmospheric Dispersion Modelling System
AERMOD	American Meteorological Society & U.S. EPA Regulatory Model
As	Arsenic
AQ	Air quality
Ba	Barium
BIOCHEM	Bologna limited area model for meteorology and chemistry
CALPUFF	California Puff Modelling System
CAM_x	Comprehensive Air Quality Model
Cd	Cadmium
CR	Cancer risk
Cr	Chromium
CFD	Computational Fluid Dynamics
CMAQ	Community Multiscale Air Quality
CMB	Chemical Mass Balance
CMEM	Comprehensive Modal Emission Model
Co	Cobalt
Cu	Copper
C-PORT	Community model for near-port applications
DOAS	Differential optical absorption spectroscopy
EDMS	Emissions and Dispersion Modelling System
Fe	Iron
FTIR	Fourier-transform infrared
HC	Hydrocarbon
HI	Hazardous index
WHO	World health organization
TH	Transport hubs
UFP	Ultrafine particles
ME-2	Multi-linear Engine 2
Mn	Manganese
MOVES	Motor vehicle emission simulator
NH_3	Ammonia
Ni	Nickel
NO_x	Oxides of nitrogen
NO_2	Nitrogen dioxide
NO	Nitrogen oxide
CO	Carbon oxide
BC	Black carbon
EC	Element carbon
GSV	Ground support vehicles
OC	Organic carbon
CI	Chloride ion
CO_2	Carbon dioxide
NH_{4+}	Ammonium ion
NO_3	Nitrate ion
SO_4^2	Sulphate ion
Sb	Antimony
TAPM	The Air Pollution Model
TEF	Toxic equivalency factor
Pb	Lead
PM	Particulate matter
V	Vanadium
VOCs	Volatile organic compounds
PEMS	Portable Emissions Measurement System
PAHs	Polycyclic aromatic hydrocarbon
PCA	Principal component analysis
PNC	Particle number concentration
PMF	Positive matrix factorisation
LTO	Landing and Take-Off
LNG	Liquefied natural gas
Zn	Zinc

concentrations in a short time-period can contribute to both short- and long-term health impacts (Cheng et al., 2011; Passi et al., 2021). In addition to commuters, workers are likely to face a higher health risk as they spend a considerable amount of time in the TH (Ben Rayana et al., 2022; Durand et al., 2021).

Each TH has specific activities that affect the local environment significantly. In airports, high pollutant concentrations were observed during take-off and landing activities, especially, ultrafine particles (UFP) emitted from the turbine engines of the aircraft (Hudda et al., 2016; Riley et al., 2016; Westerdahl et al., 2008). In ports, high pollutant concentrations were found during the manoeuvring and hostelling activity of the ship (Merico et al., 2016). In bus and train terminals, significant NO_X (NO & NO_2) and fine particulate matter ($PM_{2.5}$) emissions were observed during idling conditions (Chong et al., 2015; Y. Y. Lee et al., 2017). Though public transports modes (buses and trains) contribute very small share to the total air pollutants emissions, these transports modes contribute substantially to local and indoor AQ, while operating in TH (Williams et al., 2022).

Besides, emissions from engine combustion in airports and ports, ground support vehicles, and goods handling equipment's also contributed significant emissions locally (Hagler et al., 2021; Schürmann et al., 2007). Non-exhaust heavy metals emissions from buses and trains have gained importance recently due to the identification of carcinogenic impact on health (Harrison et al., 2021; Passi et al., 2021). Special attention has been paid to studies after 2005 in measuring and modelling pollutants such as black carbon (BC), volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), and ozone in port and airports which have serious impact on health and contribute considerably to climate change (Hagler et al., 2021; Song and Shon, 2012; Vichi et al., 2016; Xu et al., 2023).

In-depth knowledge of AQ levels and source characteristics is crucial for devising effective AQ management strategies to ensure good environmental health within and in the vicinity of THs. This paper presents a systematic literature review of studies conducted since 2005 to identify research gaps related to the types of pollutants studied, underrepresented THs, and their sources, as well as to understand the effectiveness of existing source apportionment and AQ modeling approaches in these settings. The study presents existing knowledge on various air pollutants and their typical concentrations, as well as an assessment of different methods for quantifying and detecting source contributions, and various AQ modeling methodologies, including their cost-effectiveness, efficiency, feasibility, and practicality. Previous literature review studies have summarised evidence on the most impacted pollutants, the likely health effects, the selection of measurement technologies, and the positioning of monitoring networks in THs. However, these studies did not account for the source apportionment methodologies or the various modelling techniques applied in THs. The findings from the review will provide insights into a capturing the effective and suitable methodologies to be applied for air pollution source apportionment and modelling in different THs.

2. Search strategy

A substantial number of research articles related to AQ assessment using monitoring, source apportionment and/or modelling assessments performed in, and around different THs were examined in this review. Articles published between 2005 and 2024 were considered. Database searches for each TH were performed separately. Keyword combinations for each TH setting e.g. "airport" was paired with the following words/terms "particulate", "monitoring", "dispersion modelling", "air pollution", "assessment", "effect", "prediction", "source apportionment", "measurement", "vicinity", "neighbourhood", "terminal", "platform", "nitrogen dioxide", "sulphur dioxide", and "carbon monoxide" were used in different combinations and coupled with Boolean operators ("AND", "OR", and "NOT") to optimise the search strategy. A total of 9103 research articles were accessed through Google Scholar, Web of Science, and Scopus. All duplicates were removed after the search completion. All stages of review and screening were performed by two independent researchers and discrepancies based on criteria such as article's citation index, study domain, and selection of methods were resolved by consensus and discussion. The literature search was completed in December 2024.

Studies focusing on underground train stations were omitted from this paper as the monitoring and modelling methodologies applied were different due to the indoor setting that is reflective of undergrounds, whilst airport, port, bus, and train terminals are governed more by outdoor physical and environmental characteristics. In addition, studies that adopted secondary emission factors for emission inventories and did not directly monitor or model TH conditions were excluded from this study.

2.1. Data inclusion, extraction, and analysis

Table 1 presents the inclusion and exclusion criteria of the systematic literature review. A total of 111 articles were considered. For each article, details relating to the pollutants measured, pollutant concentrations, location of the study, modeling and source apportionment techniques, and the measurement period were extracted for all four TH types. Further detail on the inclusion and exclusion criteria is included in the Supplemental Material (S.M.) in Fig. S1. For ports and airports, the review focuses on outdoor environment and the surrounding vicinity. For bus and train terminals, the review considers semi-enclosed indoor environment and the surrounding vicinity. The pollutant concentrations reported in different THs were analysed and compared. Furthermore, source apportionment techniques used in studies to quantify the contribution of TH emissions, as well as the modelling approaches employed to examine the distribution of pollutant concentrations around TH, were discussed.

Table 1
Inclusion/exclusion criteria for studies considered within the scope of the systematic literature review.

Metric	Inclusion criteria	Exclusion criteria
1.Species	Contains gaseous pollutants and PM	Contains noise & thermal comfort.
2.Data type	Contains below listed data type • Ambient air concentration in the vicinity of TH • Ambient air quality within the TH • Semi-enclosed indoor air quality in the TH • Sources associated with TH. • Emissions based on measurements • Dispersion air quality modelling • Numerical modelling • CFD modelling • Emission modelling • Regional modelling	Does not contain listed data of interest. Exclusions include e.g., • Global modelling • Estimating emission inventory (based on secondary literature emission factors)
3.Transport hub	• Commercial and general aviation • Commercial & cargo ports • Bus Terminal • Train Terminal	• Airports such as military base • Inland ports, fishing ports and docks • Roadside bus station • Intermediate train station & UG subway station
4.Distance from transport hub	Radius of 20 km from the TH – monitoring Square domain up to 50 km with TH as centre – modelling	$>$ 20 km radius from the TH – monitoring $>$ 50 km square domain with TH as centre - modelling

3. Air pollution characterisation in different TH

The geographical distribution of the AQ studies performed at THs are presented in Fig. 1. Most of these were performed in Europe followed by Northern America and China. A large number of studies has been performed assessing the AQ impacts in the vicinity of large-scale THs such as ports and airports, yet only a limited number of studies have focused on AQ in and around smaller semi-enclosed THs, such as bus and train terminals. Also, there is a significant research gap in assessing the building indoor AQ in ports and airports. Figs. 2 and 3 presents the concentrations (averaged over their study period) of major pollutants reported in the vicinity of and within the TH environments, respectively (more detailed information provided in S.M. Tables S1–S4). PM_{10}, $PM_{2.5}$, and NO_2 are commonly reported criteria pollutants across all THs, while UFP and TVOCs are measured at airports and SO_2 is measured at ports. The averaging periods of pollutants vary between studies; therefore, their concentrations were not compared to regulatory standards.

The comparison of PM concentrations at different THs show that average PM_{10} concentrations were found higher at bus terminals (36.8 $\pm$ 11.2 to- 210 $\pm$ 75.2 μg/m^3) whereas average $PM_{2.5}$ were dominant in port open areas (12.4 $\pm$ 5.4 to 147.8 $\pm$ 55.5 μg/m^3) (Cheng et al., 2012; Hagler et al., 2021; Hickman et al., 2018; Ledoux et al., 2018; Nogueira et al., 2020). High PM_{10} concentrations were observed at bus terminals in Asian and South American cities, whereas higher $PM_{2.5}$ concentrations in port studies were primarily observed in China. The high concentrations of PM_{10} in bus stations in Asian and south Asian cities were mainly attributed to resuspension of road dust due to continuous movement of buses, rather than direct exhaust and non-exhaust emissions sources (Loyola et al., 2009; Qiu et al., 2016). High $PM_{2.5}$ concentrations in port open areas was linked to road traffic emissions from inside the port in Chinese cities (Ducruet et al., 2024; Kotowska and Kubowicz, 2019).

The average NO_2 concentrations were predominantly high in train terminal investigations (52.2 $\pm$ 4.6 to 472.5 $\pm$ 50.2 μg/m^3), specifically from findings of studies performed in the United Kingdom (London, Paddington, Edinburgh & Birmingham) (Chong et al., 2015; Font et al., 2020; Hickman et al., 2018). The terminals in these cities host diesel trains which emit significant NO_2 during idling conditions (Chong et al., 2015; Font et al., 2020). Also, the terminals are semi-enclosed which further exacerbates NO_2 concentrations. NO_2 levels were found to be higher on the train station platform, followed by the concourse.

Almost all studies performed at ports reported SO_2 concentrations due to the use of high sulphur content in marine fuel used by ships. Average SO_2 levels in the studies ranged between 2.62 $\pm$ 1.0 to 78.2 $\pm$ 7.5 μg/m^3. High SO_2 levels (54.1 $\pm$ 7.7 to 78.3 $\pm$ 17.2 μg/m^3) were predominantly observed at ports in China. Low concentrations (2.62 $\pm$ 1.0 to 14 $\pm$ 3.1 μg/m^3) were observed in the studies performed in European ports after 2016. This may reflect the implementation of the EU directive allowing low-sulphur content (0.10 %) in marine fuel at berth.

A maximum sulphur content of 0.10 % in marine fuels has been enforced since 2015 in Emission Control Areas (ECAs), including the Baltic Sea, North Sea, and coastal regions of North America and the Caribbean. Outside ECAs, the sulphur limit is restricted at 0.5 %. Since 2020, the International Maritime Organization (IMO) has mandated a global sulphur limit of 0.5 %, reduced from the previous limit of 3.5 % (IMO, 2020).

Limited studies have reported on VOCs in THs, and their concentrations were considerably higher in airports (123 $\pm$ 41.1 to 973 $\pm$ 113.3 ppb). VOCs at airports are mainly released from aircraft exhaust,

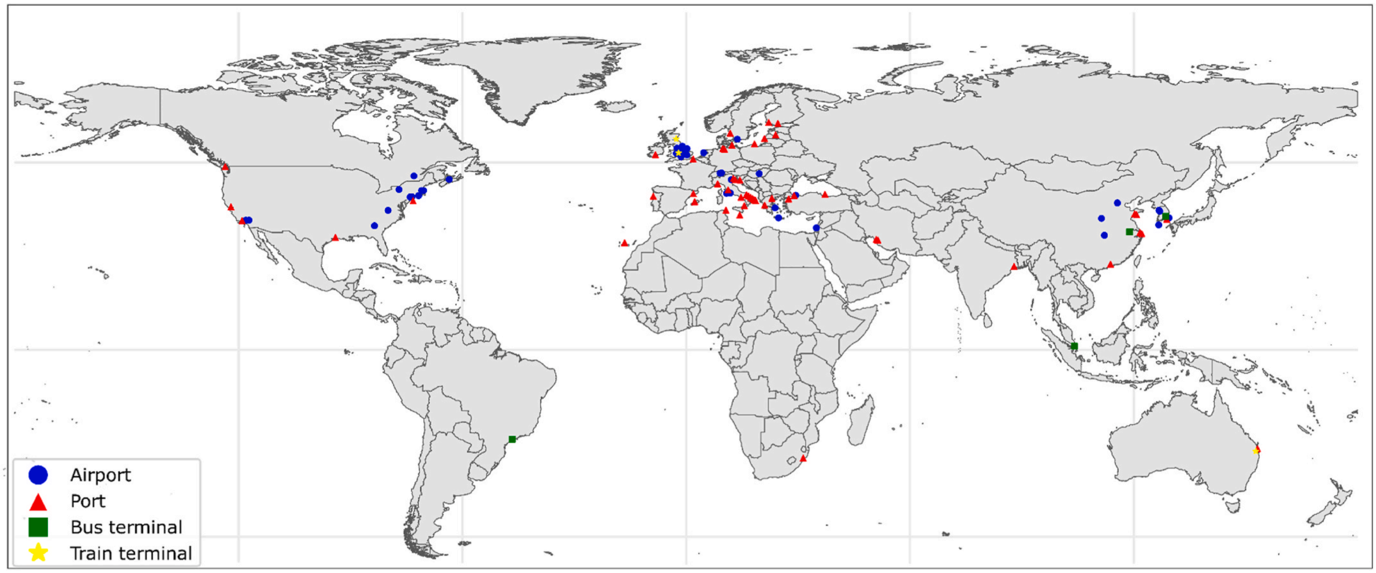

Fig. 1. Geographical distribution of air quality studies performed at THs.

fuel handling and ground support vehicles (Chen et al., 2024). The highest concentrations of VOCs were observed during aircraft idling, ignition, and taxiing conditions (Masiol and Harrison, 2014). The most abundant VOC species detected at the airport are toluene, m,p-xylene, styrene, o-xylene, and i-pentane. Toluene (14 ± 1.7 to 94 ± 21 ppb) shows the highest concentration, suggesting emissions mainly from light-duty gasoline engines. Moreover, toluene has a relatively lower photochemical reactivity compared to other VOC compounds (Fukusaki et al., 2021; Zhu et al., 2023). The presence of m,p-xylene, styrene, o-xylene, and i-pentane indicates typical fuel-related constituents. Similarly, the port area is dominated by VOC species such as toluene, acetone, m,p-xylene, n-butane, and o-xylene, primarily emitted from vehicle and ship activities (Ahmed et al., 2021).

In terms of PAH levels, only a few studies have reported their concentrations. Total PAH concentrations in the vicinity of Los Angeles Airport ranged from 37 ± 10 to 124 ± 40 ng/m^3, whereas a study conducted at Fiumicino Airport reported levels ranging from 1.0 ± 0.6 to 4.3 ± 1.8 ng/m^3 within the airport area (Vichi et al., 2016; Westerdahl et al., 2008). Benzo(b)fluoranthene, Benzo[a]pyrene, Benzo[e] pyrene, and Benzo[ghi]pyrene have been identified as the dominant PAH species in airport, primarily bound to ultrafine particles and emitted from combustion exhaust (Rodríguez-Maroto et al., 2024). At a bus terminal in Singapore, total PAH concentrations ranged from 1.6 ± 1.1 to 2.6 ± 1.4 ng/m^3, with benz[a]anthracene identified as the dominant species (Lee et al., 2022).

BC has been more extensively studied at airports compared to other THs. Reported BC concentrations at airports range from 0.34 ± 0.3 to 3.5 ± 1.4 μg/m^3, with higher levels observed near runways and terminals (Stacey et al., 2021; Targino et al., 2017). The primary sources of BC in airports are aircraft exhaust and ground support equipment. In port areas, BC concentrations range from 0.4 ± 0.3 to 2.6 ± 1.4 μg/m^3. BC, along with SO_2 and vanadium (V), can serve as tracers for apportioning ship emissions in and around ports (Hagler et al., 2021; Wang et al., 2019). More studies should focus on characterising the levels of VOCs, BC and PAHs, as well as to develop strategies for mitigating these pollutants in the THs, given their significant impacts on climate change and human health.

UFP is another pollutant consistently reported in the airport's vicinity. Elevated levels of UFP (5.0 ± 1.2 × 10^3 to 4.8 ± 1.3 × 10^6) are consistency found in the vicinity of airports compared to within airport itself, owing to landing and take-off operation (Stacey et al., 2021; Riley et al., 2016). Traces of UFP during landing and take-off activities were found up to 7.3 km downwind of the airport (Hudda et al., 2016). In bus terminals, UFP concentrations range from 2.4 ± 1.5 × 10^4 to 19.6 ± 7.6 × 10^4 particles/cm^3, with significantly higher levels in terminal areas compared to indoor environments (Cheng et al., 2012). All pollutant concentrations reported in the vicinity of a TH were considerably lower than concentrations measured within TH itself.

4. Source apportionments methods applied within and vicinity of THs

Source apportionment techniques are often used to understand the contribution of sources before and after the implementation of policy measures and technological emission control directives (Thunis et al., 2019). This evaluation can be quantified using both measurements and modelling techniques. In this section, we review the various approaches reported to detect and quantify the contribution of THs (or activity of a TH) to pollutant concentrations measured within their premises and their vicinity. Techniques applied to measurements in different THs include bivariate polar plots, data filtration techniques, regression approach, speciated receptor modelling, and the plume capture method. Table 2 presents the various techniques reported in the literature for characterising sources within and vicinity of THs.

4.1. Bivariate polar plots & data filtration technique

Bivariate polar plots are employed to discriminate between ground level sources of pollutants (emitted with little or no buoyancy (e.g., local traffic)) and sources of pollutants emitted with significant level of buoyancy (e.g., industrial, ships and aircraft plumes) (Carslaw et al., 2006). Bivariate polar plots are the extended idea of a pollution rose by incorporating the wind speed as the third variable which provides more information regarding the nature of the sources rather than the direction only (Uria-Tellaetxe and Carslaw, 2014). Bivariate polar plots are effectual in highlighting the potential sources of pollutants only when sufficient data exists from other monitoring sites to subtract background concentrations. By accounting pollutant concentration of several wind sectors affected by the similar nature of source (e.g., direction of aircraft jet plumes) and subtracting background concentration for those sectors, clear contribution of that source can be gained (Masiol and Harrison, 2015; Popoola et al., 2018).

Another quantitative method to detect pollution sources is by filtering data for a specific time period of interest such as choosing hours

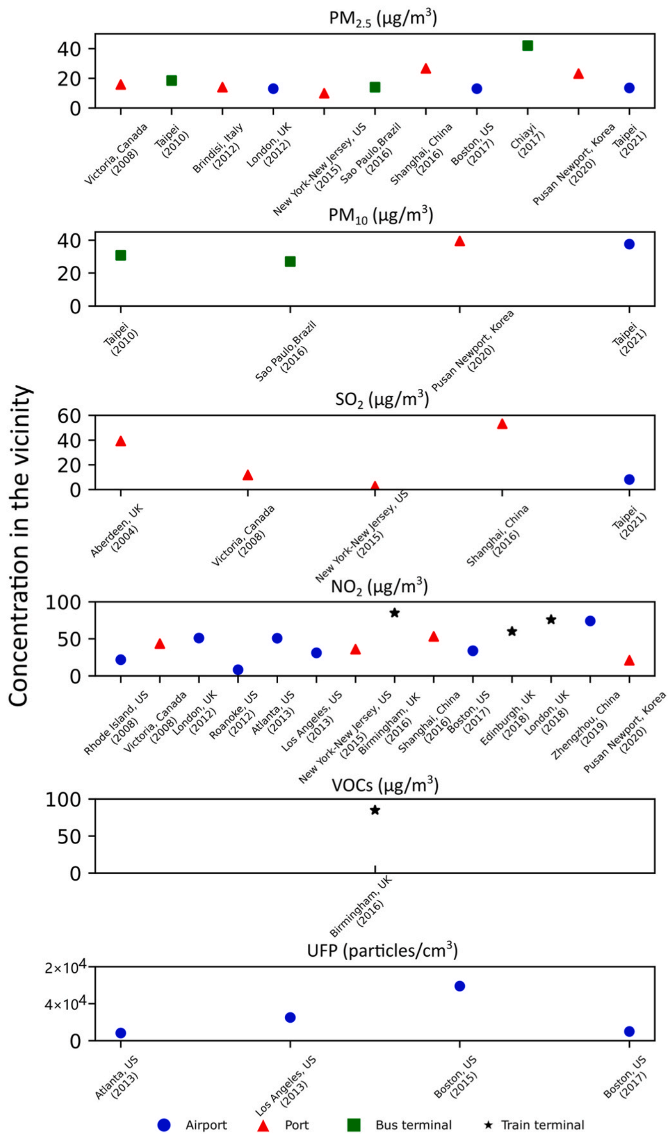

Fig. 2. Concentration of major pollutants (PM_{10}, $PM_{2.5}$, SO_2, NO_2, UFP) reported in the vicinity of TH environments (references in S.M. Tables S1–S4).

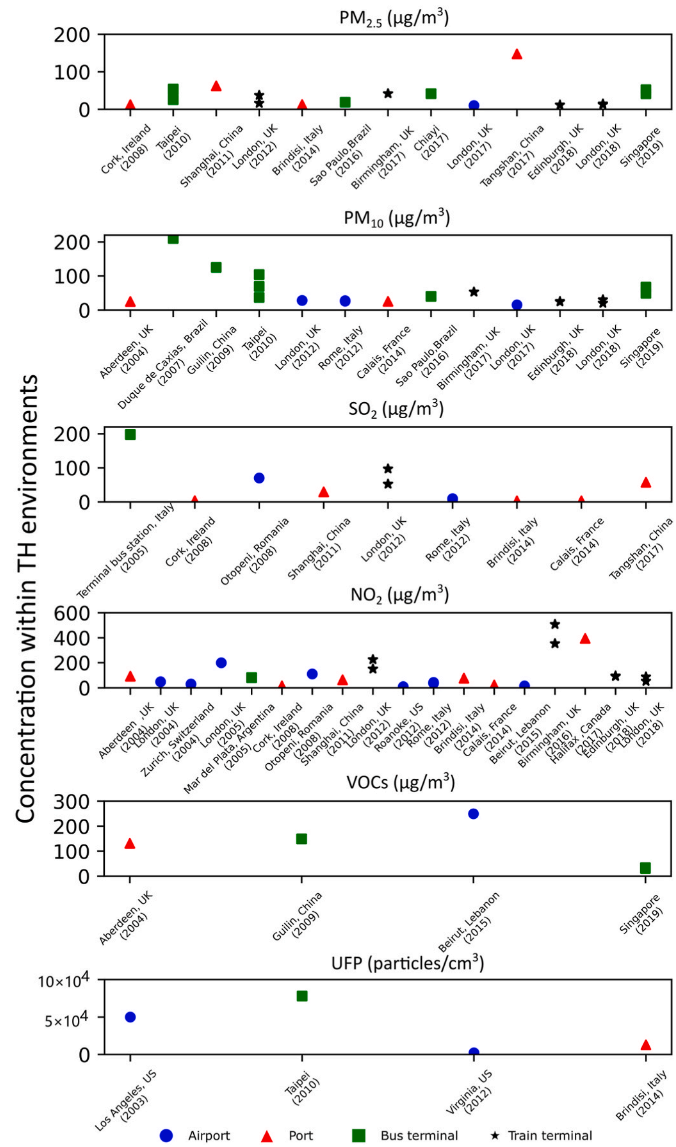

Fig. 3. Concentration of major pollutants (PM_{10}, $PM_{2.5}$, SO_2, NO_2, UFP) reported within TH environments (references in S.M. Tables S1–S4).

of the day when traffic is high, filtering data when wind direction is upwind of the measurement sites, or based on unique activity such as selecting data based on transport movements (e.g., take-off and landing of aircraft, hostelling and manoeuvring of ships, arrival and departure of buses and trains) and filtering data based on characteristics of the transport (e.g., type of engine, fuel type etc) (González et al., 2011; Hudda et al., 2016; Lelièvre et al., 2006). The average pollutant concentration corresponding to these conditions after removing the background concentration, can demonstrate the contribution of the specific source or activity (Wang et al., 2019). However, filtering on these conditions does not result in explicit quantification of sources if the influence of non-local sources is significant, which is especially challenging to disaggregate between different PM sources (Hudda et al., 2020). Wind direction becomes highly inconsistent during calm wind conditions (<1 m/s). Under such conditions, filtering data to discriminate sources becomes difficult. Some studies have restricted on the use of wind direction data under calm wind conditions (Carslaw et al., 2006; Hudda et al., 2016).

The bivariate polar plot and data filtration techniques are simple statistical methods widely used to differentiate between airport emissions and road traffic emissions in the vicinity of airports. Similarly, in port neighbourhood, these methods have been employed to distinguish port emissions from other anthropogenic activities. These techniques consistently use multiple monitoring sites measuring multiple pollutants to capture and discriminate between pollutant sources. The use of multiple sites aids in triangulating and resolving sources in greater detail around the TH. These methods assume that all activities occurring within the port or airport are treated as a single emission source during the analysis. For instance, Carslaw et al. (2006) used network of seven monitoring sites to quantify the contribution of airports to three years hourly mean concentrations of NO_2 and NO_X around the neighbourhood of Heathrow Airport, using bivariate polar plots. The study identified that airport emissions were estimated to be 27 ± 14 % of the annual mean NO_2 and NO_X concentrations in the vicinity of the airport. A study conducted in Los Angeles International Airport used landing and take-off activity data to filter the pollutant concentrations measured at seven sites around the airport. The study reported that the aircraft emitted about 4.8 ± 1.2 × 10ˆ6 particles/cm^3 (UFP) along with high NO_X (~1000 ppb) and BC (16.5 µg/m^3) concentration during take-off (Westerdahl et al., 2008).

Bivariate polar plot studies have typically employed longer monitoring periods, with data collected over more than one year, to capture a

Table 2
Methods reported in the literature to characterise the sources in the vicinity of the THs.

Methodology	Pollutant/Variables	Resolution of the data	Statistical techniques	Inference	Reference
Bivariate polar plot (8)	Gaseous pollutants, PM, wind speed & direction	15 min to 1 h	Conditional bivariate probability function	Sufficient monitoring sites to subtract the background concentrations Both high end equipment & low-cost sensors are employed	(Carslaw et al., 2006; Hagler et al., 2021; Hudda et al., 2020; Ledoux et al., 2018; Masiol and Harrison, 2015; Merico et al., 2016; Popoola et al., 2018; Xu et al., 2023)
Data filtration technique (7)	Gaseous pollutants, PM, period of take-off and landing of aircraft, period of hostelling and manoeuvring of ships, arrival and departure time of trains and buses, type of engine, fuel type, wind speed and direction	1 s to 2 min	Filtration of data on a specific period of interest (based on transport movement period, based on transport characteristics, when wind direction is upwind of measurement sites)	Sufficient monitoring sites to subtract the background levels High end equipment is required	(Carslaw et al., 2006; González et al., 2011; Hudda et al., 2016, 2020; Ledoux et al., 2018; Wang et al., 2019; Westerdahl et al., 2008)
Regression models (6)	Gaseous pollutants, PM, meteorological variables, emissions, vehicles and train count, road density, distance of road and rail from monitoring site	1 h (additive and black box model) 7–14 days (land use regression)	Additive model, land-use model, and black box models	High end equipment, diffusion tubes & low-cost sensors are employed	(Adamkiewicz et al., 2010; Carslaw et al., 2012; de Foy et al., 2021; Font et al., 2020; Han et al., 2022; Valotto and Varin, 2016)
Speciated receptor modelling (5)	PM, VOCs, PAHs	24 h	PCA/PMF/CMB/ME-2/UNMIX	Involves laboratory and require low or high-volume samplers	(Cesari et al., 2021; Hellebust et al., 2010; Masiol et al., 2016; Pirhadi et al., 2020; Vichi et al., 2016)
Plume Capture method (7)	NO_X, CO, HC, SO_2 and PM	1 s	Pollutants emissions are estimated through direct measurement or relative to CO_2 emission factor	Direct measurement requires DOAS and FTIR. Emission ratio method requires high end equipment's	(G. R. Johnson et al., 2013; Juwono et al., 2013; Klapmeyer and Marr, 2012; Merico et al., 2016; Pirjola et al., 2014; Premuda et al., 2011; Seyler et al., 2017)

wide range of dominant sources at different times at a receptor site. In contrast, data filtration techniques have been applied over shorter monitoring durations to focus on specific sources during defined time periods (e.g., emissions from landing and take-off operations at airports). These studies consistently highlight sources of NO_2 and UFPs in airport neighbourhood environments, whereas in port areas, NO_2 and SO_2 are often emphasised.

However, these methods are not effective at quantifying the dominant source of pollutants when the receptor site is influenced by a large number of sources, especially when trying to discriminate multiple emission sources within airport or port premises. Additionally, these methods are more suited for specific size range of particles (UFP range) and gaseous pollutants which arise from specific emissions. While analysing pollutants at multiple sites with high-end equipment can be expensive, the advent of low-cost monitors and effective calibration techniques has made this type of analysis more affordable in recent studies. The 17 electrochemical sensors were deployed at London Heathrow Airport over a period of five week to discriminate airport and non-local source contribution to NO_2 in the proximity of airport. The bivariate polar plots indicated that majority of the observed NO_2 concentration (75 %) (after ignoring the background concentration) arises from the emissions which are not associated with the airport sources (Popoola et al., 2018). Low-cost sensors were employed around Heuston train terminal in Dublin to discriminate and quantify the contributions of the railway station and road traffic to $PM_{2.5}$ and NO_2 levels. Data filtering based on wind orientation revealed that train station emissions were the major source of $PM_{2.5}$ (67 %), while road traffic was the major source of NO_2 (52 %) when winds were coming from the train station (Priyan et al., 2024). However, studies have not clearly specified the statistical evaluation of concentration estimated at the receptor sites compared to background sites after applying data filtration or bivariate polar plot methods. However, AQ studies have employed one-way analysis of variance (ANOVA), followed by Duncan's multiple range test, to determine whether the pollution level at one location is significantly different from that at another (Miao et al., 2024; Ipeaiyeda and Adegboyega, 2017). This approach allows for the evaluation of source contribution quantified between sites.

4.2. Regression models

Regression models are another simplified method for identifying major sources in the TH. Unlike dispersion models, regression models lack an analytical expression, but they allow for the exploration of detailed relationships between pollutants and variables such as traffic and emission rates, which significantly impact pollutant concentrations. These models are used to assess potential reductions in pollutant levels when the magnitudes of these variables are decreased. However, they cannot quantitatively estimate the individual contributions of sources (e.g., airport and road traffic) to the pollutant levels. Studies using regression models have consistently highlighted sources of NO_2 at TH. Like bivariate polar plots and data filtration techniques, regression models are also more effective at discriminating gaseous pollutant sources. Han et al. (2022) adopted a generalised additive model to analyse the impact of airport related emissions on hourly measured NO_X concentrations in Xinzheng International Airport, China. This study used hourly airport emission data (take-off, landing, ground taxi, ground support equipment) together with meteorological and environmental data and found that 13 % of the NO_X concentrations were explained by the airport activity emissions. Adamkiewicz et al. (2010) applied a land use regression (linear model) to identify the impact of airport and local traffic on NO_2 concentrations (7- and 14-day measurements using diffusion tubes) in proximity to the airport for three months (644 measurements). NO_2 concentrations were modelled against land use variables (such as traffic density, road length, and distance to road, terminal, and runway) and the model demonstrated that local traffic has a strong influence on the NO_2 concentrations. Studies related to generalised additive models have modelled pollutants with an R^2 of 0.41–0.60, while studies using linear models have shown lower performance, with an R^2 of 0.30–0.32. Using linear models poses difficulties as many variables are unexplained and confidence in these models is fairly modest.

Linear regression models and generalised additive models have frequently been used in studies, but recent studies have increasingly adopted machine learning models such as random forests, stochastic gradient boosting, and boosted regression trees due to their superior predictive power (Font et al., 2020; Pan et al., 2023). These models can handle a mix of variables, including both categorical and continuous types, efficiently manage missing data, and are resistant to outliers in the variables.

A study conducted in Edinburgh Waverly and London King's Cross railway stations modelled hourly $PM_{2.5}$ and NO_2 concentration (4-week measurements) and activity data of trains (such as train fuel type, train schedule, platform distance). Model enabled the prediction of individual contributions from different train types using a random forest model, with an R^2 between 0.50 and 0.80. The model identified a strong association between pollutants and diesel trains. Furthermore, it predicted that reducing the number of diesel trains would decrease $PM_{2.5}$ concentrations by an average of 0.18–0.48 μg/m^3 per train and NO_2 concentrations by 8.6–23.7 μg/m^3 per train. (Font et al., 2020). Both generalised additive model and machine learnings models are better in explaining the variables than linear models. Additionally, the studies have used longer monitoring period for outside environment (3–12 months) and shorter monitoring period for semi-enclosed indoor environment (7–30 days).

4.3. Speciated receptor modeling

The above methods are less effective in quantifying PM and VOCs sources when a receptor site is influenced by a large number of sources, especially within TH premises. However, PM and VOCs sources can be effectively quantified even at extremely complex sites with a wide range of differing sources using the speciated receptor modelling approach. Besides emissions from aircraft, ships and trains, this method can be used to quantify emissions from ground service equipment, domestic heating, heavy-duty trucks, and non-combustion sources such as soil and road dust, brake wear, and tire wear within as well as in the vicinity of the TH.

Speciated receptor modelling aims at analysing the physical (size distribution) or chemical characteristics of particles. This helps in identifying potential chemical or size markers and statistically matching them to sources signature, and finding their contribution (Hopke, 2016; Shanmuga et al., 2021). Over the decades, receptor models have become effective tools in managing AQ. The receptor models reported in AQ studies include Principal Component Analysis (PCA), Positive Matrix Factorisation (PMF), Chemical Mass Balance (CMB), Unmix, and Multi-linear Engine 2 (ME-2), with more than 1000 studies applying these methods (Hopke, 2016). However, source apportionment studies conducted in and around THs have not employed Unmix and ME-2.

The study conducted in Brindisi port, Italy characterised $PM_{2.5}$ based on its chemical composition (elements, ions, and organic content) and used PCA to identify the sources of $PM_{2.5}$ sampled for 93 days. The study identified ship emissions, sea salts, crustal dust, vehicular emissions, and secondary aerosols as the main source of $PM_{2.5}$ (Cesari et al., 2021). Hellebust et al. (2010) utilised a PMF model to quantify the sources of $PM_{2.5}$ using gaseous pollutants, $PM_{2.5}$ organic fraction and sulphate particles as factor variables sampled for four months in the harbour of Cork, Ireland. The study identified fuel oil combustion (31 %) as the major contributor followed by vehicular emissions (19 %) and domestic solid fuel burning (14 %). A study conducted in Shenzhen, China, collected VOCs samples at 110 sites using steel canisters, quantifying 22 VOCs species at each site. PMF model identified airport emissions as the major VOCs source in and around Shenzhen Airport (Zhu et al., 2023).

This approach relies solely on PM and VOCs chemical composition collected at the receptor site, without the need for emission rates, traffic flow data, background levels, or meteorological information. Studies using the receptor modelling approach have employed both shorter and longer monitoring periods (1–5 months) to effectively discriminate between sources. However, this approach is expensive, requiring sophisticated sampling and laboratory instruments. Hence, single site is mostly preferred in the studies.

PMF and ME-2 model has been the preferred model in recent years as they resolves factor contribution without significant negative values (Comero et al., 2009) and are more accurate than CMB and UNMIX for sources quantification. In contrast, PCA is limited to identifying important sources at a receptor site (qualitative). The advantage of using a PMF and ME-2 model are improved accuracy and effectiveness in identifying and quantifying the individual contributions of different sources and hence is more suitable for complex environments.

In these models, source profiles are used either as input data (e.g., in CMB) or as reference profiles for comparison with model outputs (e.g., in PMF, UNMIX, ME-2, and PCA). Many countries have developed their own country-specific source profiles; however, these profiles are often limited in their applicability to THs. In such cases, the USEPA speciate database can be utilised. The speciate database provides an extensive range of source profiles specifically for airport-related activities including aircraft exhaust, ground idling and thrust operations, landing and take-off cycles, and nonroad ground support equipment as well as for port-related sources such as propulsion engines, auxiliary engines, marine vessel boilers, and ground support equipment. For instance, Jeong et al. (2017) used USEPA speciate 4.3 marine vessel database and CMB model to quantify the contribution of ship emissions powered by heavy fuel oil at the port of Busan, South Korea.

Furthermore, receptor modelling studies were mainly focused on quantifying the sources of PM in ports and airports vicinity, with no studies have been found for train and bus terminals.

4.4. Plume capture method

The plume capture method is another approach used to evaluate the effectiveness of policy implementations and technological emission control measures, as well as to estimate emission factors for modelling purposes. Pollutant emission rates from sources such as aircraft, trains, and ships are measured while they are moving by capturing their plume. These emission rates are directly measured from the plume with ground-based stations or indirectly estimated by measuring CO_2 concentrations from the plume using the emission ratio method.

Differential Optical Absorption Spectroscopy (DOAS) and Fourier-transform infrared (FTIR) absorption spectroscopy are the common ground-based instruments used to measure the emissions rates of gaseous pollutants from moving sources (Premuda et al., 2011). DOAS measures different trace gases along an optical path in a narrow band absorption structure in the visible and UV spectral region, while FTIR measures the trace gases in the infrared region (Schürmann et al., 2007)

Emission rates by emission ratio method is computed by using Eqns. (1) and (2).

$$ER_X = \frac{X - X_{bg}}{CO_2 - CO_{2,bg}} = \frac{\Delta X}{\Delta CO_2} \quad \text{(Eqn.1)}$$

$$EF_X = ER_X \cdot \frac{M_X}{M_{CO_2}} \cdot EF_{CO_2} \quad \text{(Eqn.2)}$$

where.

ER_X is the emission ratio for pollutant X;

X_{bg} and $CO_{2,bg}$ are the background concentrations for pollutant X and CO_2, respectively.

EF_X is the emission factor for the pollutant X;

M_X and M_{CO_2} are the molecular mass of the pollutant X and CO_2, respectively

EF_{CO_2} is the emission factor of the CO_2.

These methods do not require long monitoring periods (typically between 7 days and 60 days is reported), and the emission estimates reflect real-world conditions. Premuda et al. (2011) carried out two months of measurements using DOAS to estimate NO_2 and SO_2 emissions from large and medium-sized ships passing through the channels in two ports (Stazione Marittima and Porto Marghera, Italy). The study found that NO_2 and SO_2 emissions ranged between 4.64 and 5.49 g/s and 1.47–2.63 g/s respectively, with the larger ship emitting less than the medium ships. A study performed at Brisbane, Australia adopted an emission ratio method to quantify pollutant emissions ($PM_{2.5}$, PNC, SO_2, NO_X) from diesel trains entering and leaving the local port. The sampling was carried out for 7 days with the continuous measurement of pollutants and CO_2. EF values of $PM_{2.5}$, PNC, SO_2 and NO_X were found to be (1.1 ± 0.5) g/kg fuel, (17.1 ± 1) × 10^{16}/kg fuel, (14 ± 0.4) g/kg fuel, (28 ± 14) g/kg fuel, respectively (Johnson et al., 2013).

In the emission ratio method, measurements are taken close to the source to capture the plume, typically 100–125 m from the runway at airports, 15–100 m from the channels in ports, and 9–10 m from trains. The measurements are conducted at a specific height, ensuring no obstructions exist between the source and the instrument. Additionally, measurements are taken upwind to account for background concentrations.

Emission rates measured using DOAS and FTIR can be conducted from much greater distances (1–6 km). These methods often yield more accurate estimates than the emission ratio method. However, DOAS and FTIR instruments are expensive and require an elevated, fixed station without any obstructions between the instruments and the source plume. These instruments are applicable only to gaseous pollutants (SO_2 and NO_2).

5. Air quality modelling approaches applied at THs

As summarised in Table 3, AQ modelling is primarily used in studies to evaluate model results against measurements, forest AQ, apportion TH emissions to local AQ, and assess the reduction in pollutant concentrations achieved through the implementation of policy and technological measures (Gao and Zhou, 2024). The commonly reported AQ models in the THs includes Gaussian models, Eulerian & Lagrangian models and CFD (Gao and Zhou, 2024; Thunis et al., 2016).

5.1. Gaussian models

The Gaussian plume model assumes that pollutants are continuously emitted, representing them as a single expanding plume over time (Johnson, 2022). The pollutant species concentration is directly proportional to the emission rate of the source, diluted by the wind velocity at source (Gibson et al., 2013). The dispersion of the pollutant is calculated using the standard deviation associated with the gaussian distribution (Holmes and Morawska, 2006). Gaussian-derived models, which include the American Meteorological Society and U.S. Environmental Protection Agency Regulatory Model (AERMOD), the Community model for near-port applications (C-Port) and the Atmospheric Dispersion Modelling System (ADMS), are typically employed for AQ research at airports and ports.

AERMOD is a grid-less model has potential of predicting sources impact from 1 to 50 km away. Model has been used to understand the impact of point and volume pollution sources at local scale, including

Table 3
Models reported in the literature to characterise air quality at THs.

Model Type	Model	Study number	Domain	Spatial resolution	Time resolution	TH	Pollutant	Performance Indicator (NMB)	References
Gaussian	AERMOD	14	Local scale (up to 40 km)	100m–200m	Hourly-Annual	Airport	PM_{10}	−2.31 to 11 %, R^2: 0.62–0.78	(Abrutytė et al., 2014; Buccolieri et al., 2016; Cesari et al., 2018, 2021; Cohan et al., 2011; Ekmekçioğlu et al., 2020; Gibson et al., 2013; Groma et al., 2018; Henry-Lheureux et al., 2021; Isakov et al., 2017; Kose et al., 2022; Koulidis et al., 2020; S. Kuzu, 2018; S. L. Kuzu et al., 2021; Makridis and Lazaridis, 2019; Mandal et al., 2021; Merico et al., 2019; Mokalled et al., 2022; Popoola et al., 2018; Sabatino et al., 2011; Song and Shon, 2012; Sorte et al., 2019)
							$PM_{2.5}$	−2.2 to 10.4 %, R^2: 0.68–0.81	
							NO_X	5–13 %	
							CO	0.29–6.6 %, R^2: 0.52–0.72	
						Port	NO_X	−11 to −65 %, R^2: 0.4–0.45	
							$PM_{2.5}$	24–36 %	
	ADMS	6	Local scale (up to 13 km)	45m–230m	Hourly	Airport	NO_2	5–20.4 %, R^2: 0.33–0.65	
							$PM_{2.5}$	−4 to 16.1 %	
							O_3	7–10 %, R^2: 0.65–0.79	
	C-PORT	2	Local scale (up to 10 km)	10m–40m	Hourly	–	–	–	
Eulerian	TAMP	3	Local scale (up to 28 km)	250m–500m	Hourly-Annual	Airport	NO_2	−11 to −38 %, R^2: 0.16–0.25	(Ramacher et al., 2019, 2020; Tang et al., 2020)
							$PM_{2.5}$	−7 to −54 %, R^2: 0.25–0.71	
						Port	NO_2	5 To 15 %, R^2:0.73–0.79	
	CMAQ	5	Regional scale	1 km–27km	Hourly-Monthly	Airport	$PM_{2.5}$	−53.9 to 82 %	(Rissman et al., 2013; Song et al., 2015; Yang et al., 2018; J. Zhang et al., 2021; Zhou et al., 2020)
							SO_4	−57.4 to −57.6 %	
							NO_3	5.4–6.1 %	
							O_3	3.1–20.6 %	
	CAMx	2		6 km–36km	Monthly	–	–	–	(Bo et al., 2019; Merico et al., 2017)
	WRF-Chem	1		3 km	Monthly	Port	$PM_{2.5}$	−14.4 to −21.3 %, R^2: 0.59–0.66	Chen et al. (2017)
Lagrangian	SPRAY	2	Local scale (up to 50 km)	100m-1km	Hourly	Airport	NO_X	−36 to −89 %	(Gaeta et al., 2016; Kontos et al., 2017; Murena et al., 2018; Pecorari et al., 2016; Poplawski et al., 2011)
							CO	−35 to −60.8 %	
							HC	−44 to −134 %	
	CALPUFF	3	Local scale (up to 30 km)	100m–200m	Hourly	Port	SO_2	30–52 %	
							$PM_{2.5}$	36–69 %	
							NO_2	−44 to 14 %	
CFD		2	Microscale (up to 10m)	Centimeter	Per second	–	–	–	(Yoo et al., 2022; Yu et al., 2022)

the sources which emit benzene, hydrogen cyanide, SO_2 and PM (Gibson et al., 2013; Kalhor and Bajoghli, 2017). Similarly, ADMS (Viz. ADMS-airport & ADMS-urban) can model pollutant concentrations across a range of scales, from street level to city-wide level. ADMS-airport is the most used model in the airport environment, while ADMS-urban is the model mostly employed in the port environment to model the pollutants concentrations in its vicinity (Cesari et al., 2018, 2018, 2018; Mokalled et al., 2022). ADMS-airport includes all the features of ADMS-urban, additionally it incorporates the airport specific sources such as air traffic, ground support vehicles, auxiliary power units and other less-defined airport sources. Additionally, ADMS-airport incorporates jet model which captures the near-field dispersion of the jet exhaust emission during take-off and landing activities (Voogt et al., 2023). Both AERMOD and ADMS incorporates advanced modules such as sulphate chemistry, NO_x – NO_2 chemistry (Holmes and Morawska, 2006).

The plume transport model, AERMOD and ADMS cannot process the variable calm wind condition (Cohan et al., 2011; Makridis and Lazaridis, 2019). A common way to deal with this problem, is to replace the meteorological condition with allowable wind speed that is representative of the physical processes. Wind speed is generally chosen as smallest non-zero velocity which can be handled by model and wind directions are equally chosen for all directions for calm winds. If the calm wind condition periods are of low percentage, these periods can be excluded in the modelling to prevent overestimation of results. For instance, Cohan et al. (2011) selected a smallest non-zero velocity of 1 knot as a cut-off value and assumed wind direction equally probable in all direction to account for calm and variable winds in AERMOD. The study highlighted roadway emission as the major local pollution compared to ship emissions in the ports of Los Angeles and Long Beach.

C-port is another dispersion modelling system which can estimate emissions from the port terminals and helps in assessing the AQ impacts from ports (Isakov et al., 2017). The c-port models the primary pollutants such as SO_2, NO_X, $PM_{2.5}$, CO, formaldehyde, benzene, acrolein, and acetaldehyde (CMAS, 2016). The model represents multiple activities in the port including rail, road, and terminal activities. The model's algorithm for the point and area sources are similar to AERMOD, and the line-source algorithm is consistent with US EPA C-line model. However, this algorithm is simplified for computational efficiency, as C-port is a web-based application. The C-port model currently uses data from 21 seaports in the U.S. and incorporates the local meteorology of these locations (C-PORT, 2016). Hence, its applicability is limited for use in other port locations worldwide and hence model is not further reviewed in the article.

The study domains used in the studies performed in port and airport ranged from 6 × 9 km to 40 × 40 km, with grid resolutions between 100 m and 200 m. Both AERMOD and ADMS models can predict hourly pollution levels; however, if only annual or monthly emissions are available, emissions can be parameterised based on traffic data and assume a steady release of emissions. Vutukuru and Dabdub (2008) parameterised emissions such that 70 % occur between 8 a.m. and 8 p.m. and 30 % between 8 p.m. and 8 a.m. at the port. Weekend emissions are set to 50 % of the weekly average.

Estimating hourly pollution levels is computationally intensive for larger domain, thus some studies have restricted the stimulation for shorter period rather than for whole year (Cohan et al., 2011; Vutukuru and Dabdub, 2008). All the emissions sources in both port and airport are treated as an area source (Gibson et al., 2013). However, there is limitation in AERMOD in treating sources like landing and take-off (LTO) of aircraft as area sources. The emissions during LTO are assumed to be uniformed disturbed over a defined area with a specific vertical spread (plume rise). In AERMOD, area sources do not allow the treatment of plume rise, which restrict the accurate prediction of buoyant plume rise of jet exhaust. In contrast, ADMS-airport incorporate the treatment of plume rise accounting for both buoyancy of jet exhaust as well as momentum (Popoola et al., 2018). Despite its limitation, the studies conducted at airports using AERMOD have shown good agreement between modelled and measured values, with mean biases of 5–13 % for NO_x, −0.29 to 6.6 % for CO, −2.2 to −10.4 % for $PM_{2.5}$ and −2.31 to −11 % for PM_{10}. Similarly, ADMS-airport also demonstrated with good agreements with the measurements with a mean bias of 5–20.4 % for NO_2, -4 to 16.1 % for $PM_{2.5}$ and 7–10 % for O_3. AERMOD is widely employed in ports environments, with the mean bias error of −11 to −65 % for $PM_{2.5}$ and 24–36 % for NO_X. Model tends to exhibit lower errors (−11 to 24 %) in areas closer to port compared to farther away locations.

Overestimation of NO_X near the port and airport is observed from both AERMOD and ADMS-airport, respectively. This may partly be due to the absence of chemical reactions that act as sinks for NO_x in the model. Similarly, underestimation of PM is observed, which could be attributed to the underrepresentation of the secondary organic aerosol component of PM, likely caused by larger uncertainties in the PM emission inventory. Both models showed improved results with the incorporation of the photochemistry module. Additionally, the inclusion of background concentrations improved the models results.

Similar to aircraft plume, ship manoeuvring in ports also requires plume rise treatment, however, manoeuvring emissions are relatively lower compared to hoteling emissions, which are the most significant among port emissions. As a result, manoeuvring emissions have a lesser impact on the model results and are often ignored during modelling.

5.2. *Eulerian & Lagrangian models*

Eulerian dispersion modelling uses conversation of mass equation for a given species of concentration C. A stationary grid of reference is presumed, with the dispersion phenomena being computed as a concentration field with respect to the reference grid (Collett and Oduyemi, 1997). The physical conditions in the reference grid are treated as turbulent, so that dependant variables are composed of an average component (Collett and Oduyemi, 1997). Lagrangian dispersion modelling differs from Eulerian counterparts is that pollutant dispersal is stimulated in relative to the shifting reference grid (Collett and Oduyemi, 1997; Rissman et al., 2013). Eulerian & Lagrangian dispersion models identified in the airport and port studies includes TAPM, CALPUFF, SPRAY, CAMx, WRF-Chem and CMAQ (Chen et al., 2017; Gaeta et al., 2016; Merico et al., 2017; Ramacher et al., 2020a). These models are typically employed to understand the process of air pollution including the transport of pollutants, deposition, and chemical transformation in regional scale (Gao and Zhou, 2024; Ramacher et al., 2020b).

CAMx, CMAQ, TAMP and WRF-Chem are three-dimensional Eulerian multi-scale models that support grid nesting and multi-model integration, capable of simulating complex physical and chemical interactions among atmospheric pollutants (Gao and Zhou, 2024). TAPM uses grid based Eulerian dispersion model for regional scale with Lagrangian particle mode to near source concentrations (Ramacher et al., 2019; Ramacher et al., 2020a). While these models are primarily used at the regional scale, they can be configured with smaller grid sizes (e.g. 250 × 250 m) in nested domains to focus on specific areas such as ports or airports. However, these finer-resolution nested domains require boundary conditions provided by a larger, coarser surrounding domain. Sub-grid analysis is performed to understand the airport or port contribution to the pollutant concentrations (Ramacher et al., 2020b). For instance, Ramacher et al. (2019) used TAPM to evaluate the effects of local shipping emissions on AQ with five nested grid system ranging from 10 × 10 km to 250 x 250m. The chemical boundary conditions were taken from the CMAQ stimulation on a 4 km × 4 km grid. The study reveals a significant impact of local shipping on local NO_2 concentrations, contributing between 5 and 15 % of the annual grid mean NO_2 concentration.

CALPUFF is Lagrangian puff multi-species model capable of stimulating the effect of varying meteorological conditions and longer-range transport effect on pollutants transformation and removal (Kontos et al., 2017; Poplawski et al., 2011). SPRAY is a Lagrangian particle mode model used in studying dispersion and deposition of the non-reactive emissions of passive pollutants (Gaeta et al., 2016; Pecorari et al., 2016). Unlike other regional-scale models, CALPUFF and SPRAY can calculate dispersion from multiple sources at the microscale with a smaller grid size (100 m × 100 m) without requiring a coarser surrounding domain. Murena et al. (2018) assessed the impact of cruise ship emissions on Naples, Italy, using CALPUFF with a 36 × 24 cell grid and 200m cell spacing to model cruise ship emissions. The results show a low correlation between the fixed monitoring stations data and the simulations, suggesting that the contribution of NO_2 emissions from cruise ships is insignificant within the Naples metropolitan area. Pecorari et al. (2016) analysed the effects of meteorology on aircraft exhaust dispersion at Marco Polo Airport in Venice employing SPRAY with a 500 × 500 cell grid and 100 m spacing to assess spatial dispersion of HC and CO during LTO cycles. The study highlighted aircraft taxiing as the most impactful during operations, with specific meteorological events (low wind speed and inversion conditions) causing increased HC and CO concentrations in the airport neighbourhood.

Among Eulerian models, TAPM and WRF-Chem tend to predict values close to measured concentrations in the port vicinity (TAPM, mean bias: 5–15 % for NO_2; WRF-Chem, mean bias: −14.3 to −19.8 % for $PM_{2.5}$). However, Eulerian models tend to produce larger mean bias errors near airport vicinities (TAPM, −7 to −54 % for $PM_{2.5}$ & −11 to 38 % for NO_2; CMAQ, 53.9–82 % for $PM_{2.5}$). The large mean bias near airports can be attributed to several factors, including the lack of precise information on aircraft timing and trajectories, the limited number of emitters used to represent the various modes of aircraft emissions, uncertainties in aircraft engine emission estimates, and inadequate representation of plume characteristics. Few studies have incorporated advanced plume treatments in their models, where emissions from aircraft sources are represented as Gaussian puffs (Bo et al., 2019; Yang et al., 2018). A chemical mechanism "CMAQ-APT" is utilised to simulate reactions both within the puff as well as within the grid cells. However, the inclusion of this process did not result in a significant improvement in the model's performance. The insufficient availability of measurements of aircraft plumes makes it challenging to accurately represent real-world plume characteristics in the model.

WRF-CMAQ model showed reasonable agreement with measured ozone concentrations in the airport environment, attributed to the substantial emissions of VOCs and NO_x (Song et al., 2015). The mean bias error between modelled and observed values ranged from −3.1 % to 20.6 %.

Like Eulerian models, Lagrangian models also exhibits with larger mean bias error for airport vicinities than port vicinities. SPRAY is commonly used to understand the impact of airport emissions on local NOx, HC, and CO concentrations in airport's neighbourhood. The mean bias error for pollutants modelled using SPRAY in the airport vicinity range from −36 % to 89.6 % for NO_x, −35 % to −60.8 % for CO, and −44 % to −134 % for HC. The model performance slightly improved when considering the background concentration. SPRAY model is effective in modelling the physical dispersion of pollutants but does not account for chemical transformations. However, the atmosphere around airports is a complex environment with hundreds of chemical reactions occurring, which could attribute to significant errors in the model results. While CALPUFF is commonly employed in port to understand effect on local SO_2, NO_2, and $PM_{2.5}$. The mean bias error for pollutants modelled using CALPUFF in the port vicinity range from 30 % to 52 % for SO_2, 36 %–69 % for $PM_{2.5}$, and - 44 %–14 % for NO_2. Inadequate representation of plume characteristics in the CALPUFF model, particularly building downwash of the plume is attributed to underestimation of concentration (Poplawski et al., 2011). Also, representing ship emission as line source is not the best choice, the ship emissions should be represented as a series of volume sources.

Gaussian model results showed reasonable agreement with ground-level measurements compared to Eulerian and Lagrangian regional models in airport vicinities. However, Eulerian models (TAPM and WRF-Chem) performed slightly better in predicting pollutants near ports. Additionally, the Eulerian model exhibited better agreement with ground-level measurements at locations farther from the port than the gaussian model, as it is better equipped to handle complex terrain and non-steady-state meteorological conditions typical of coastal areas.

For regulatory compliance purposes, when the focus is on near-field impacts, Gaussian models are more suitable due to their computational efficiency. ADMS-airport is more appropriate for airport environment than the AERMOD. However, if the study involves modeling secondary pollutants or long-range transport, Eulerian are more appropriate, as they can account for chemical reactions, temporal variability, and complex dispersion dynamics.

5.3. *Computational fluid dynamics (CFD)*

CFD tools has become an important part of environmental modelling. CFD models are based on the Navier-Stokes equations and can accurately stimulate the turbulent flow dynamics while accounting the complexity of the built-up environment explicitly (Mumovic et al., 2006). CFD models are more suitable for microscale environments due to limitations such as being restricted to non-reactive pollutants, negligible thermal effects, concentration of specific hour depending solely on the emissions within the modelling domain, NO_2 and NO_X ratio, and meteorological condition at that hour (Martín et al., 2024). CFD models for AQ modelling in TH have been only applied in bus terminals, as the semi-enclosed nature of bus terminals reduces computational demands compared to other TH (Yoo et al., 2022; Yu et al., 2022).

Yoo et al. (2022) employed CFD to simulate the dispersion of NO_2 originating from a semi-enclosed bus station terminal to optimise the placement of an air purification system. The study involved the construction of a comprehensive model that incorporated the geometric features of the bus station and utilised the Re-Normalised Group (RNG) k-epsilon turbulence model to predict the distribution of NO_2. The findings revealed that the effectiveness of the air cleaning system depends on the specific combination of inlet and outlet locations. Similarly, Yu et al. (2022) employed CFD to investigate the dispersion of CO from a bus exiting a station. The study focused on assessing the impact of bus stop platform type and passenger location on individual exposure to pollution.

6. Study limitations & future directions

6.1. *Study limitations*

The systematic literature review only considered articles published between 2005 and 2024, thus a small number of pre-2005 articles may have provided added insights for the review. Also, this paper limited its inclusion criteria to published articles in scientific journals, thus findings from grey literature e.g., government reports etc., were not included in the review. Additionally, comparing different monitoring and modelling methodologies is difficult as studies were heterogenous (different methods, pollutants, study populations, etc.) and had different study objectives.

However, modeling and source apportionment methods can be transferable between sites, their applicability depends on the type of pollutant and source characteristics. Data filtration, regression models, and bivariate polar plot techniques are more appropriate for gaseous pollutants such as NO_2 and SO_2, particularly when these originate from specific, localised sources. In contrast, speciated receptor modeling is more suitable for PM and VOCs, which typically originate from multiple sources. This method is not transferable to sites focused on assessing NO_2 and SO_2 sources. The plume capture method is specifically suited for assessing pollutants emitted from moving transportation sources.

While AQ modeling approaches are transferable between sites, the results are often inconsistent, as each model behaves differently due to variations in their underlying physical and chemical mechanisms. Gaussian models are more suitable for smaller domains and for assessing near-field impacts, whereas Eulerian models are more appropriate for modeling secondary pollutants and the long-range transport of pollutants.

Source evaluation should start with simple methods such as data filtration, regression analysis, bivariate polar plot or Gaussian models to assess potential sources and the complexity of the site. Based on the complexity and pollutants studied, other source apportionment methods such as speciated receptor modeling and plume capture method should then be prioritised.

6.2. Future directions

Based on the literature reviewed, local-scale THs, such as bus and train terminals, are underrepresented in current research (Fig. 4). Therefore, it is recommended that future research should focus on: (i) characterising PM and gaseous pollutant sources in the vicinity of these terminals to understand their contribution to ambient conditions; ii) investigating the impact of idling, fuel consumption, traffic and micro-meteorology on pollutants concentration; (iii) categorising UFP contributions from terminal related activities (idling, arrival, and departure) at these terminals; (iv) distinguishing PM sources of exhaust and non-exhaust emissions at these terminals; and (v) employing AQ modelling within train terminals to understand semi-enclosed indoor air pollution effects.

Moving forward, as AI and digital twins revolutionise air pollution monitoring and forecasting, future research should focus on demonstrating the impact of AI on AQ monitoring and management at THs. Future studies should integrate deep learning models with the Internet of Things to enhance health awareness and improve pollution exposure management in and around THs. This includes issuing AQ warnings, implementing emission control measures, and modifying traffic management plans during periods of high pollution. Additionally, more research should explore the combination of low-cost sensors with AI-based calibration, as this approach offers a cost-effective solution for managing AQ.

7. Conclusions

This review synthesises existing air quality (AQ) literature to define the current state-of-the-art and identify research gaps concerning the effectiveness of monitoring and modelling approaches in and around transport hubs (THs).

While numerous studies have assessed air pollution impacts near large-scale THs, such as ports and airports, comparatively few have focused on smaller, semi-enclosed settings like bus and train terminals. This represents a significant research gap, particularly regarding indoor AQ within port and airport buildings.

PM_{10}, $PM_{2.5}$, and NO_2 are commonly reported criteria pollutants across all THs, while UFP and TVOCs are measured at airports and SO_2 is measured at ports. Notably, PM_{10} concentrations tend to be higher at bus terminals, $PM_{2.5}$ dominates in port areas, and NO_2 levels are elevated in train terminals, especially those serving diesel-powered trains. Further research is needed to characterise pollutants such as volatile organic compounds (VOCs), black carbon (BC), and polycyclic aromatic hydrocarbons (PAHs), given their substantial health and climate impacts.

Analytical techniques such as bivariate polar plots, data filtration, and regression models are frequently employed to assess pollutant sources within and around THs. These methods are favoured for their simplicity, resource efficiency, and effectiveness in source discrimination. Studies often incorporate meteorological variables and background concentrations alongside historical AQ data. Speciated receptor modelling is commonly applied at sites with significant particulate matter (PM) pollution and complex emission profiles. Plume capture methods, particularly the emission ratio approach, are used to estimate real-world emission rates, relying primarily on standard AQ instruments and reliable CO_2 emission factors.

Gaussian dispersion models are predominantly used for large-scale THs, such as airports and ports, and generally show good agreement with ground-level measurements. Compared to Eulerian and Lagrangian models, Gaussian models offer more reliable results when emissions, background concentrations, and secondary chemistry (e.g., nitrate and sulphate formation) are included. However, uncertainties in emission inventories, pollutant interactions, and meteorological conditions can affect model accuracy. Increasing the number of measurement sites within or around THs can enhance model calibration and validation, leading to more accurate predictions and better source attribution.

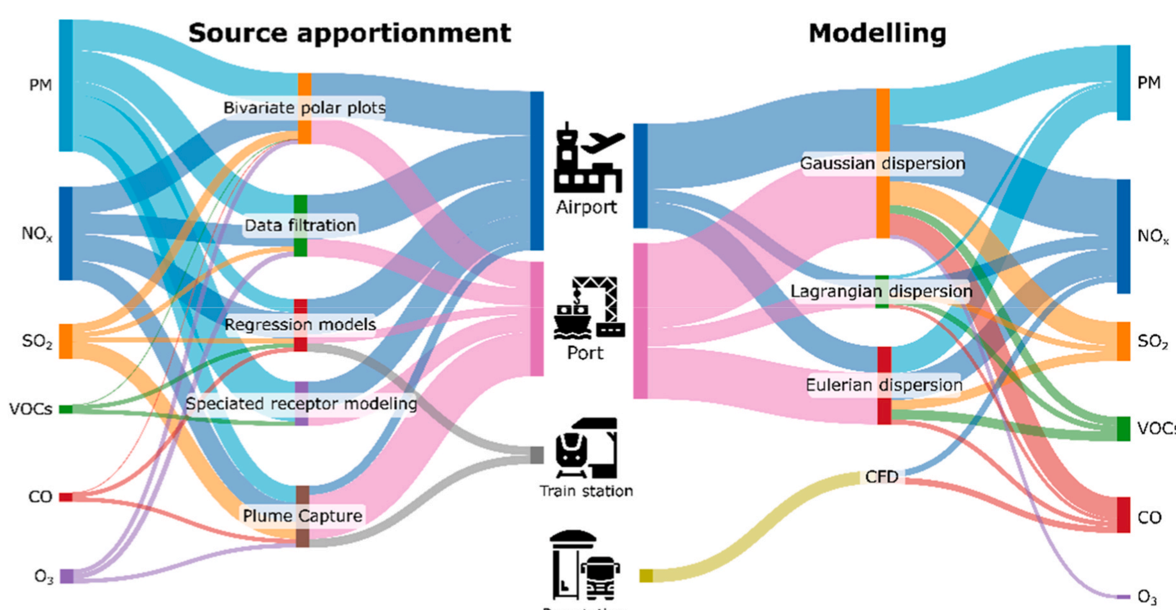

Fig. 4. Breakdown of studies that have focused on applying monitoring and modelling methodologies to evaluate air quality in different THs.

Computational fluid dynamics (CFD) models have been applied to simulate pollutant dispersion within bus stations. The enclosed nature of these terminals reduces computational demands relative to other THs. In contrast, AQ modelling for train terminals remains limited, highlighting the need for further research to determine the most suitable modelling approaches for these environments.

There are identified knowledge gaps that require further investigations in this field, with the role AI offering a potential avenue to better leverage data and support improving air quality in TH settings.

CRediT authorship contribution statement

Shanmuga Priyan: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization. **Yuxuan Guo:** Writing – review & editing, Writing – original draft, Visualization, Formal analysis, Conceptualization. **Brian M. Broderick:** Writing – review & editing. **Brian Caulfield:** Writing – review & editing. **Aonghus McNabola:** Writing – review & editing. **Margaret O'Mahony:** Writing – review & editing. **John Thornes:** Writing – review & editing. **John Gallagher:** Writing – review & editing, Supervision, Resources, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Shanmuga Priyan R reports financial support was provided by Environmental Protection Agency Ireland. Yuxuan Guo reports financial support was provided by Environmental Protection Agency Ireland. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apr.2025.102709.

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