AIR POLLUTION CONFERENCE BRAZIL
CMAS SOUTH AMERICA
COMMUNITY MODELING AND ANALYSIS SYSTEM

DEVELOPMENT OF AUTOMATED COMPUTATIONAL TOOLS FOR EMISSION INVENTORY AND REAL-TIME ATMOSPHERIC DISPERSION MODELING

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Abstract: Atmospheric dispersion modeling is an important tool to assess the impacts of air quality associated with emissions from activities and operations of different types of industrial facilities. This type of study depends on several operational and meteorological conditions. Atmospheric dispersion studies conducted currently aim mainly to meet the requirements of environmental agencies, providing a static air quality scenario based on historical meteorological conditions. Emission rates from source activities are mandatory input data for the execution of atmospheric dispersion models. There are different methodologies for estimating these rates, ranging from real-time measurements in stacks from industrial processes to the use of emission factors, such as those provided by the U.S. EPA AP-42 Compilation of Air Pollutant Emission Factors. However, estimating emissions based on these factors can be complex, as it requires an extensive set of information about the emission source, does not represent the operational variability of the source, and requires more time for the analysis and consolidation of documentation. In this context, the application of the AERMOD model using historical meteorological data and fixed emission rates can limit the ability to obtain rapid and effective responses to support decision-making in industrial operations. In addition, this approach may involve high software licensing costs, as well as manual collection and processing of meteorological data. To address this gap, Aires Environmental Services developed online platforms for real-time atmospheric dispersion modeling and emission source inventory management: AiresFlow and Aires Emission. By using public and private data platforms, it was possible to integrate the system with up-to-date databases, enabling results with high temporal resolution. In online mode, AiresFlow can perform minute-by-minute modeling for periods of up to three days, making it suitable for the analysis of industrial processes and for rapid response to operational occurrences. AiresFlow is integrated with Aires Emission, which provides a complete library of U.S. EPA AP-42 emission factors within the browser, including all chapters, sections, and listed industrial processes. Aires Emission automatically calculates emission rates and updates the emission source database used by AiresFlow. Therefore, AiresFlow and Aires Emission contribute to air quality management by providing rapid responses to industrial facilities through continuous modeling. These tools enable fast diagnosis of industrial processes presenting anomalies, thereby improving process monitoring while supporting compliance with environmental requirements.
Keywords: real time, atmospheric dispersion, AERMOD, air quality.

INTRODUCTION

Atmospheric dispersion modeling is an important tool for assessing the impacts on air quality associated with atmospheric emissions from various industrial activities and operations. Conducting dispersion studies requires integrating detailed information on emission sources, operational characteristics, and meteorological conditions, as well as applying mathematical models capable of representing the processes of pollutant transport and dispersion in the atmosphere. However, most atmospheric dispersion studies traditionally rely on historical meteorological conditions and fixed emission rates, resulting in a static representation of air quality. Furthermore, the collection, processing, and consolidation of the necessary data can require significant processing time, limiting the ability to obtain rapid responses to support decision-making in industrial operations. In this context, Aires has developed the AiresFlow and Aires Emission computational platforms, integrated with the AERMOD model and the U.S. EPA's AP-42 emission factor database, with the goal of automating the management of emissions inventories and enabling real-time atmospheric dispersion modeling (U.S. Environmental Protection Agency, 2004, 1995). These tools enable greater agility in evaluating operational scenarios, contributing to the monitoring of industrial processes and the improvement of air quality management.

METHODS

The AiresFlow platform integrates atmospheric emissions estimation and dispersion modeling into an automated workflow. Emission rates are derived from US EPA AP-42 emission factors (based on Web-

FIRE). Meteorological data are acquired from multiple sources using prioritization and fallback mechanisms, ensuring complete hourly time series: surface data (METAR/ASOS) from local stations and the Iowa Environmental Mesonet (Iowa State University), supplemented by forecasts (Google Weather, Tomorrow.io, and NCEP GFS 0.25° via Unidata THREDDS); and upper-air data (radiosondes) from the University of Wyoming and IGRA/NOAA. The observations are converted to the SAMSON format and processed by AERMET, generating surface (SFC) and profile (PFL) files. Topography is handled by AERMAP (SRTM elevation), defining the receptor grid and elevations. Dispersion is simulated using the US EPA AERMOD regulatory model (Gaussian, steady-state, hourly resolution), resulting in concentrations (μg/m³) per receptor and per hour (POSTFILE), visualized as plumes and time series. The platform was developed in TypeScript/React (frontend) and Python (Django/DRF and FastAPI), with asynchronous processing via Celery/Redis and data persistence in PostgreSQL/PostGIS and AWS S3.

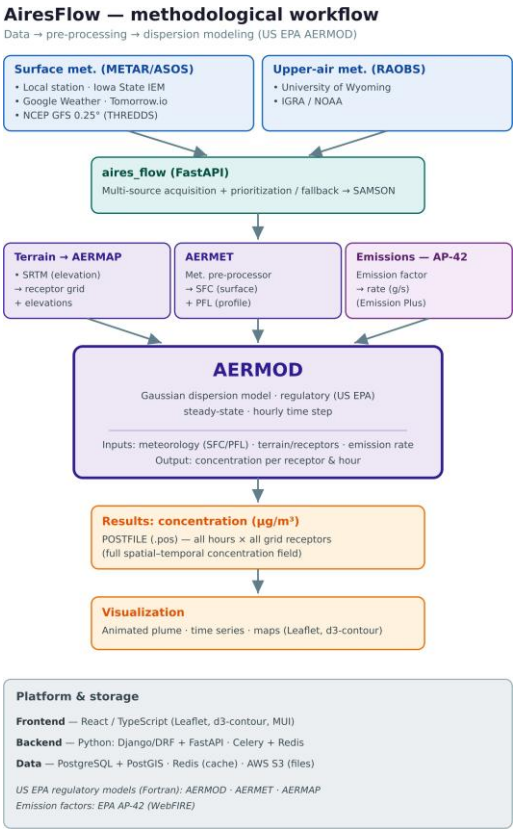


Figure 1. Integrated workflow of the AiresFlow platform, including meteorological preprocessing, emission estimation, dispersion modelling, and result visualization.

FINDINGS AND ARGUMENT

AiresFlow has developed a web-based platform that fully automates the AERMOD/AERMET-based atmospheric dispersion modeling workflow, from meteorological data acquisition to the georeferenced visualization of plumes.

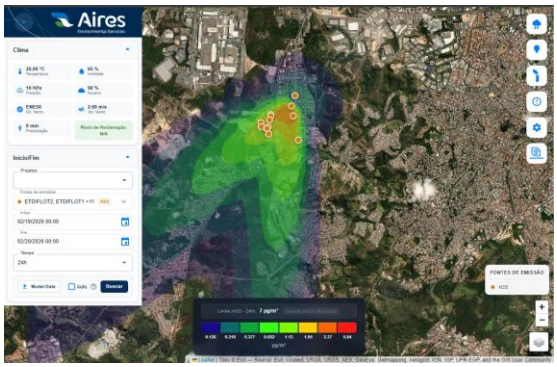


Figure 2. Atmospheric dispersion plume generated on the AiresFlow web platform.

With the following results:

- **End-to-end automation:** From a single request, the system generates the input file (.INP), runs AERMET (Stages 1 and 2/3) and AERMOD, and returns the results—eliminating the need for manual preparation of meteorological data.
- **Meteorological data with guaranteed fallback:** SAMSON surface series assembled through parallel aggregation of multiple sources in order of priority—local station METAR/Iowa State (148 stations in Brazil) Google Weather API GFS/THREDDS (always available).
- **Synthetic altitude profiles:** in the absence of radiosondes, estimation of vertical profiles using three methods (standard logarithmic, Batchvarova e Gryning, Driedonks).
- **Analytically derived parameters:** dew point (Magnus-Tetens), wet-bulb temperature (Stull, 2011), and cloud cover (clarity index), allowing for complete data sets even with limited stations.
- **Georeferenced visualization:** GeoJSON contours on an interactive map with isolines (IDW + d3-contour) and time-series animation.
- **Forecasting mode:** dispersion modeling for forecasting, with a forecast horizon of up to 72 hours (3 days).

CONCLUSIONS

AiresFlow has integrated the entire atmospheric dispersion modeling cycle using AERMOD/AERMET into a single web platform, automating everything from the multi-source acquisition of meteorological data—with a fallback mechanism that ensures the continuity of simulations—to the georeferenced visualization of plumes. Its ability to operate in prognostic mode, automatic comparison with regulatory limits, and auditing capabilities provide the tool with technical value, regulatory compliance, and reliability for decision-making, establishing it as a scalable solution for atmospheric impact assessment and air quality management.

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