# Development and Validation of a 3D CFD Software for Atmospheric Dispersion Analysis of Chemical Releases

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## 1. Introduction

In nuclear power plants and large-scale energy facilities, various chemicals such as ammonia and chlorine are used for cooling water treatment, auxiliary systems, and chemical handling processes. In the event of an accidental release, these substances can disperse into the atmosphere, potentially posing severe risks to facility integrity, personnel safety, and surrounding areas. Therefore, accurate prediction of chemical dispersion behavior is essential for nuclear safety assessment and emergency response planning.

## 2. Background and Configuration of CESARE

To address this need, a new software system named CESARE has been developed. CESARE integrates a three-dimensional CFD solver based on OpenFOAM with multiple supporting modules, including:

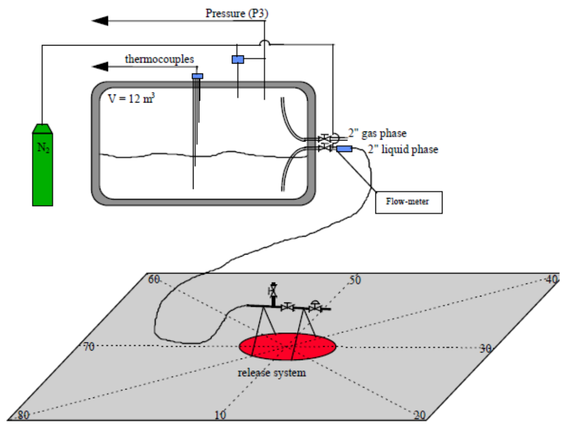
(1) Chemical database and leak source calculation
(2) Meteorological data integration
(3) CAD-based automatic geometry and mesh generation
(4) Jet and atmospheric dispersion analysis, fire modeling, and explosion risk assessment

This system enables a unified framework to simulate the complete chain of accidental scenarios, from chemical release to dispersion, combustion, and explosion assessment
Fig. 1 illustrates the overall configuration of the CESARE software, showing its modular structure and integrated workflow.

## 3. Description of the INERIS Experiment

For validation of the dispersion analysis capability, the large-scale ammonia dispersion experiments conducted by INERIS (Institut National de l'Environnement Industriel et des Risques) in France were selected as reference cases[1]. Among these, Experiment No.1 was chosen, in which liquefied ammonia was released into an open field environment and concentrations were measured at multiple distances along the plume centerline and its surroundings.


Fig. 1. Configuration of the CESARE software




(a) Release point diagram

(b) Typical ammonia plume
Fig. 2 INERIS Experiment

Fig. 2(a) shows the schematic of the release point, while Fig. 2(b) presents a typical ammonia plume generated during the experiment. These figures provide a clear depiction of the experimental setup and the observed dispersion cloud.

## 4. Validation Methodology and Results

Prior to applying CESARE, preliminary simulations

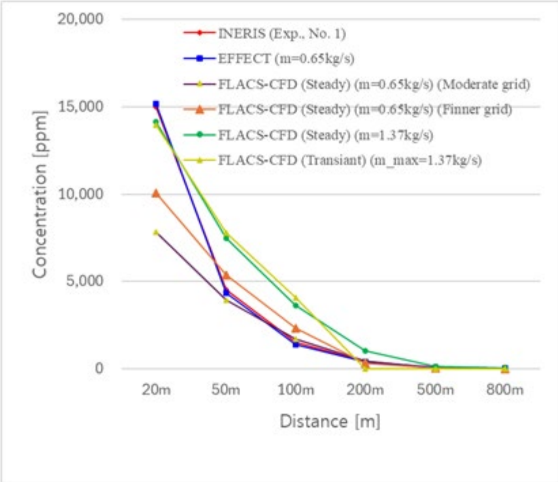
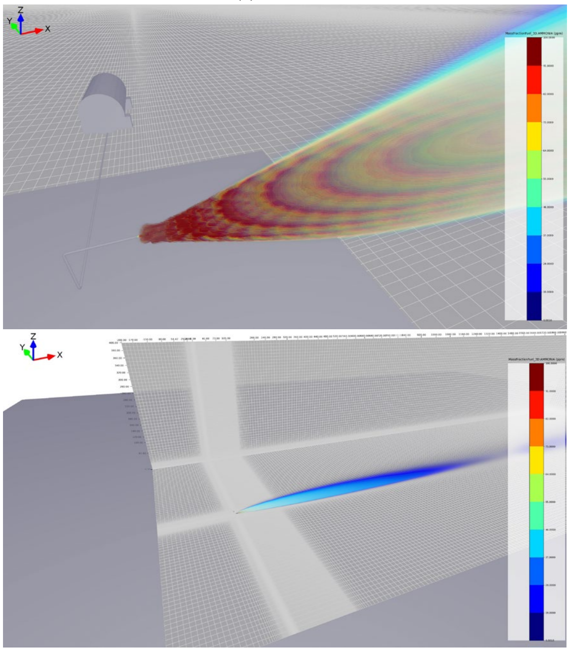



Fig. 3. Comparison of concentration vs. distance between experiment, EFFECT, and FLACS-CFD

(a) EFFECT



(a) FLACS-CFD

Fig. 4. Concentration distribution

were performed using established models and commercial codes under the same INERIS Experiment No.1 conditions(wind speed: 5m/s):

(1) EFFECT model[2]: A semi-empirical dispersion model for concentration prediction.
(2) FLACS-CFD[3] A commercial CFD software widely used for large-scale gas release and explosion analysis

The predicted results were compared against experimental measurements. Fig. 3 presents the concentration versus distance for the experiment, EFFECT, and FLACS-CFD, providing a quantitative benchmark for model performance.

In addition, Fig. 4 shows the two&three-dimensional concentration distributions obtained from EFFECT (Fig. 4a) and FLACS-CFD (Fig. 4b). These visualizations enable a direct qualitative comparison of the plume spreading and dilution predicted by the two methods.

The analysis results revealed that the EFFECT model reproduced reasonable concentration levels near the release point but underestimated plume dilution at longer distances. In contrast, FLACS-CFD provided results more consistent with the experimental trends, particularly in terms of plume width and concentration decay over distance.

## 5. Conclusion and Future Work

A three-dimensional CFD-based software, CESARE, was developed to predict atmospheric dispersion behavior of hazardous chemical releases in nuclear power plants and large industrial facilities. As a first step toward validation, the INERIS ammonia dispersion experiment was analyzed using EFFECT and FLACS-CFD, and their results were compared with experimental data.

In the next phase, CESARE will be applied to the same INERIS conditions. The results will be systematically compared with EFFECT, FLACS-CFD, and experimental data to verify the predictive performance of CESARE. Through this process, CESARE will be established as a reliable tool for nuclear safety assessment and chemical accident emergency planning.

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