



“Gheorghe Asachi” Technical University of Iasi, Romania



NUMERICAL SIMULATION OF LIQUID AMMONIA LEAKAGE DISPERSION CONSIDERING LIQUID-GAS TRANSITION

Bo Zhang^{1*}, Yun Long¹, Fei Xiao², Ying Liu³

¹State Key Laboratory of Chemical Safety, College of Mechanical and Electronic Engineering,
China University of Petroleum (East China), Qingdao 266580, P.R. China

²Gas Transmission Management Department, PetroChina Southwest Oil and Gasfield Company, Chengdu, 610200, P.R. China

³Dan F. Smith Department of Chemical Engineering, Lamar University, Beaumont, TX, 77710, USA

Abstract

Liquid ammonia release accidents occur periodically, drawing significant attention to the study of ammonia release and dispersion consequences. Traditional consequence simulations using computational fluid dynamics (CFD) often simplify the liquid ammonia leakage source as gaseous ammonia, overlooking the critical liquid-gas transition process. To address this limitation, the present study employs the Euler-Euler approach to model the liquid-gas transition, with the Mixture model selected as the multiphase flow model. The mass and energy transfer between liquid and gaseous ammonia are incorporated into Fluent through a user-defined function (UDF) based on the Lee model. A case study of liquid ammonia release and dispersion in a refrigeration workshop is conducted to investigate the consequences of leakage under the liquid-gas transition model. The analysis also considers the influence of ventilation shutters installed on the workshop walls. The simulation results are compared with those obtained from a simplified single-phase model based on vapor ammonia concentration distribution. The comparison reveals that neglecting the liquid-gas transition leads to exaggerated predictions, including a wider dispersion range and altered concentration distributions, which may result in misleading risk zones for ammonia leakage consequences. The proposed method offers a more realistic and engineering-relevant approach for quantitative risk assessment (QRA) in scenarios involving liquid-gas transition processes.

Key words: computational fluid dynamics, liquid ammonia release, liquid-gas transition, Lee model, ventilation shutters

Received: October, 2023; Revised final: January 2025; Accepted: August, 2025

* Author to whom all correspondence should be addressed: e-mail: zhangbo@upc.edu.cn