INTRODUCTION
Prompt estimation of the atmospheric dispersion characteristics of hazardous materials following a release over an industrial site is of crucial importance for the emergency responders. Quick, yet accurate predictions of the contaminated area are required.

parameters:
• the real time wind field
• building topography
• composition-decay characteristics of the initially emitted species.

The aim is to provide emergency responders with sufficiently accurate and rapid data in order to allow them to decide the emergency measures to be taken.

The location is an industrial site near the city of Bourges in France. The release scenario is a pool fire of ethanol of 100 m² area. The duration of release is taken equal to 1 hour.

QUIC (Pardyjak and Brown 2001) atmospheric dispersion modeling system is used.

CHEMICAL KINETICS OF AN ETHANOL POOL FIRE
parameters:
• equivalence ratio of 4
• pressure is 1 atm.
• the temperature of the flame is 1400K (Weckman and Strong )

Thomas empirical correlation (Rew et. al. 1997) gives the size of the reaction zone as:

\[ D = 42 \left( \frac{m^2}{\rho_f \cdot g \cdot D_f} \right)^{0.6} \]  

- L is the flame height, is computed to be 0.08 m for a 0.073 m² pool
- \( \rho_f \) is the density of air at ambient conditions (kg.m⁻³)
- g is the gravitational acceleration (m.s⁻²)
- D is the pool diameter (m)
- \( m^2 \) the mass burning rate of fuel is taken to be 0.020 kg.m⁻².s⁻¹ for ethanol.

CHEMKIN-PSR (Glarborg et al. 2011) model with Dagaut (1992) mechanism used for kinetic simulations (Table 1).

ATMOSPHERIC DATA
The mesoscale atmospheric flow model WRF is used for atmospheric conditions at 15th of each month for the year 2012 (Skamarock et al., 2008) for the Bourges area using the Research Data Archive at the National Center for Atmospheric Research (Figure 1).

DECAY RATES
The atmospheric degradation rates of the products of ethanol fire are necessary for modelling their atmospheric dispersion. The photochemical oxidation rate coefficients for the reaction with OH radicals ( and NO₂ radicals and ozone reactions for 1-butene) are taken from IUPAC database.

The atmospheric lifetimes of the released compounds are given by:

\[ \tau_{OH} = \frac{1}{k_{OH} + c_{OH}} \]  

- \( k_{OH} \) are the bimolecular rate constants for the reaction of OH radicals with the compounds
- \( c_{OH} \) is the OH concentration that is taken as 2x10⁸ and 0.5x10⁸ (molecules/cm³) during daytime and night time, respectively (Lu & Khalil, 1992).

In the case of 1-butene:

\[ \frac{1}{\tau_{OH}} = \frac{1}{c_{OH}} + \frac{1}{c_{C_2H_4}} + \frac{1}{c_{C_2H_2}} + \frac{1}{c_{C_2H_5}} \]

where \( c_{C_2H_4} = 0.5x10^{10} \) (molecules/cm³) and \( c_{C_2H_2} = 1x10^{11} - 2x10^{10} \) (molecules/cm³) during daytime and night time, respectively (Geyer 2000; Padasaine et al., 2006).

1-butene has the shortest lifetime: 210 minutes (daytime).

Toluene is more stable with its shortest lifetime equal to 1200 min.

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