PREDICTING THE FORMATION AND THE DISPERSION OF TOXIC COMBUSTION PRODUCTS FROM THE FIRES OF DANGEROUS SUBSTANCES

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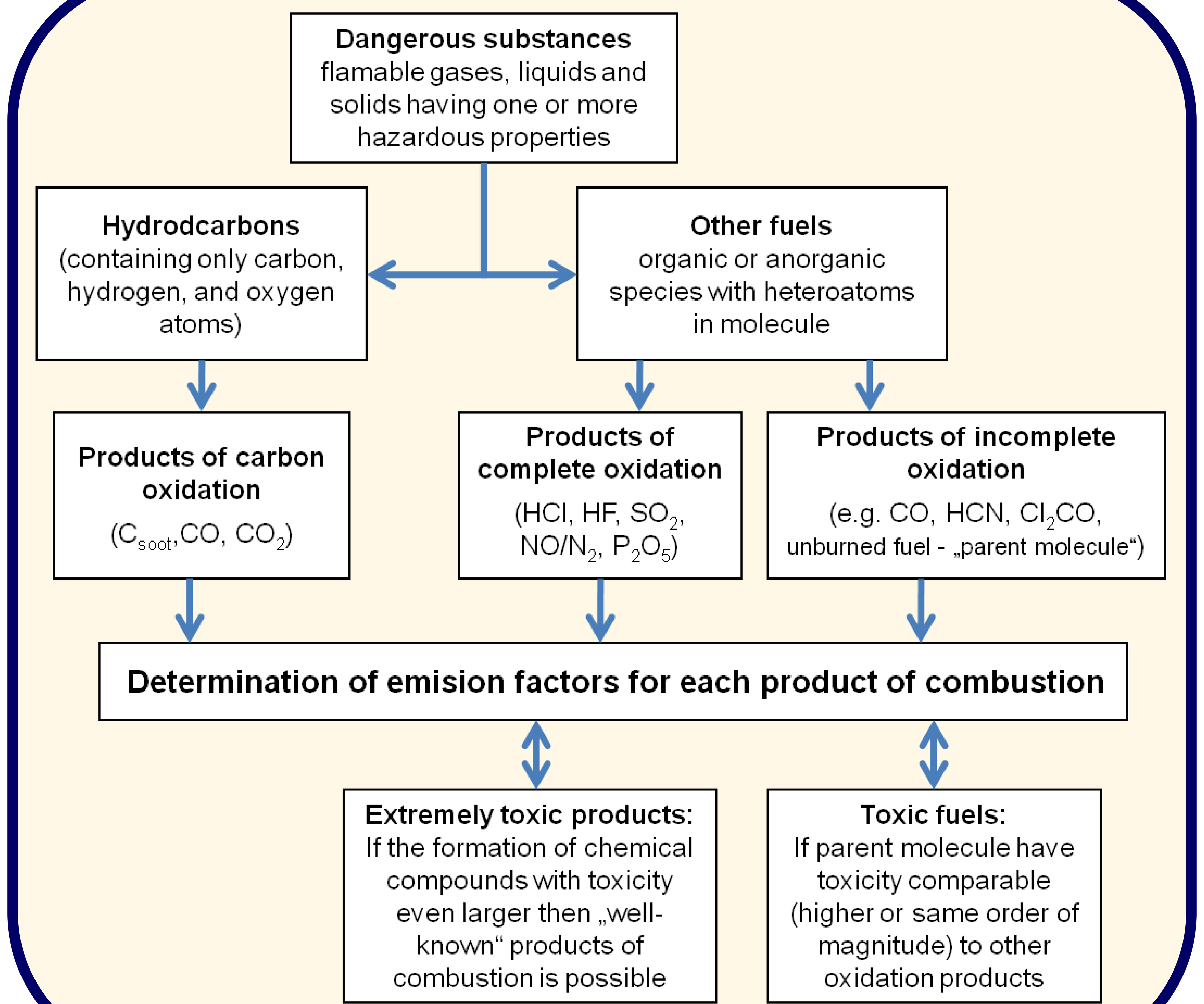
ABSTRACT:

Natural events, such as wildfires, lightning or earthquakes represent a frequent trigger of industrial fires involving dangerous substances. Dispersion of smoke plume from such fires and the effects of toxic combustion products are one of the reference scenarios expected in the framework of major accident prevention. Nowadays, tools for impact assessment of these events are rather missing. Detailed knowledge of burning material composition, atmospheric conditions, and other factors are required in order to describe quantitatively the source term of toxic fire products and to evaluate the parameters of smoke plume. Nevertheless, an assessment of toxic emissions from large scale fires involves a high degree of uncertainty, because of the complex character of physical and chemical processes in the harsh environment of uncontrolled flame. Among the others, soot particle formation can be mentioned as still being one of the unresolved problems in combustion chemistry, as well as decomposition pathways of chemical substances.



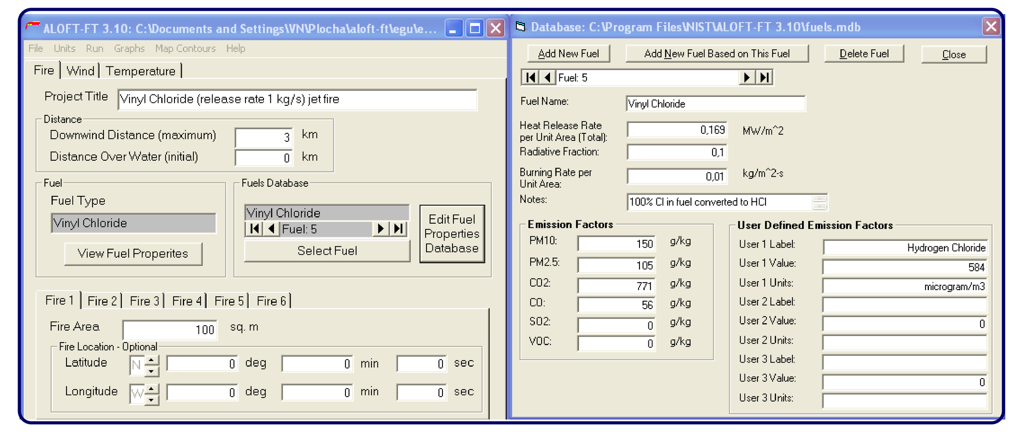
More then 150 dangerous chemicals identified (with qualitative assignement of possible combustion products):

Name	Phase (293K)			Formula	Molar mass	Number of atoms									Combustion products					
	l	g	s			C	H	O	F	Cl	S	N	Br	…	A) HCl	B) HBr	C) HF	D) HX	F) NO_x	…
Acetamide, N-phenyl-	0	0	1	$CH_3.CO.NH.C_6H_5$	135	8	9	1	0	0	0	1	0		0	0	0	0	1	
Acetone cyanohydrin	1	0	0	$(CH_3)_2.C(OH)(CN)$	85	4	7	1	0	0	0	1	0		0	0	0	0	0	
Acetonitrile	1	0	0	$CH_3.CN$	41	2	3	0	0	0	0	1	0		0	0	0	0	0	
Acetyl bromide	1	0	0	$CH_3.CO.Br$	123	2	3	1	0	0	0	0	1		0	1	0	0	0	
Acetyl chloride	1	0	0	$CH_3.CO.Cl$	78.5	2	3	1	0	1	0	0	0		1	0	0	0	0	
Dichlorethene	1	0	0	CHCl:CHCl	97	2	2	0	0	2	0	0	0		1	0	0	0	0	
Vinil chloride	1	0	0	H2C:CHCl	62.4	2	3	0	0	1	0	0	0		1	0	0	0	0	

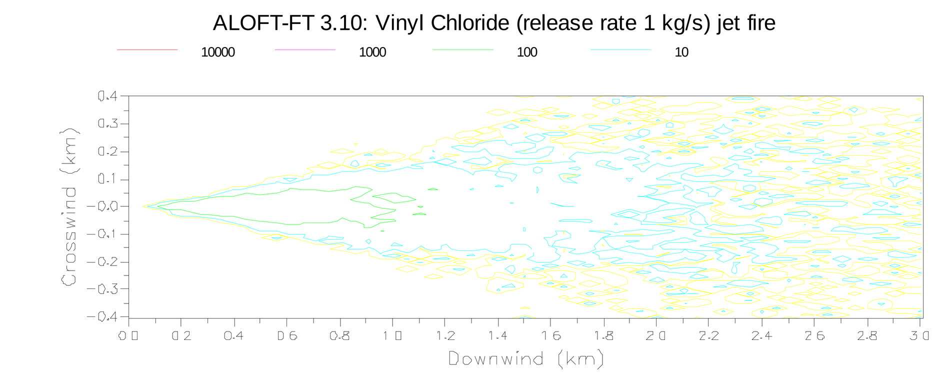
Emission factors for each combustion product were estimated (using simplifying assumtions) based on the balance of carbon and other elements (heteroatoms) present in the molecule of fuel.

Fuel:	C_2H_3Cl				
Atoms in fuel molecule:		C	H	Cl	
		2	3	1	
		12	1	35,45	
Molar weight of C in fuel molecule:		24	3	35,45	
Molar weight of fuel molecule:		62,45			
Products	C(s)+CO2+CO+HCl				
$F_{carbon,fuel}$	Mass fraction of carbon in fuel	0,384			
$F_{carbon,soot}$	Mass fraction of carbon in soot	1,000			
$F_{carbon,CO}$	Mass fraction of carbon in carbon monoxide	0,429			
$F_{carbon,CO2}$	Mass fraction of carbon in carbon dioxide	0,273			
$F_{chlorine,fuel}$	Mass fraction of chlorine in fuel	0,5676541			
$F_{chlorine,HCl}$	Mass fraction of chlorine in hydrogen chloride	0,9725652			
E_{soot}	Emission factor of soot particles	0,150	=>	150	g/kg
η_{soot}	$E_{soot}/F_{carbon,fuel}$	0,390			
$G_{soot,C}$	$\eta_{soot}*F_{carbon,soot}$	0,390			
η_{CO}	$\eta_{CO}=0.0014+(0,37*\eta_{soot})$	0,146			
$G_{CO,C}$	$\eta_{CO}*F_{carbon,CO}$	0,062			
$G_{CO2,C}$	$1-(G_{CO,C}+G_{soot,C})$	0,547			
η_{CO2}	$G_{CO2,C}/F_{carbon,CO2}$	2,006			
$G_{HCl,Cl}$	Yield of hydrogen chloride from chlorine in fuel	1,000			
η_{HCl}	$G_{HCl,Cl}/F_{chlorine,HCl}$	1,028			
E_{CO}	$\eta_{CO}*F_{carbon,fuel}$	0,056038	=>	56,03803	g/kg
E_{CO2}	$\eta_{CO2}*F_{carbon,fuel}$	0,7710675	=>	771,06754	g/kg
E_{HCl}	$\eta_{HCl}*F_{chlorine,fuel}$	0,5836669	=>	583,66693	g/kg

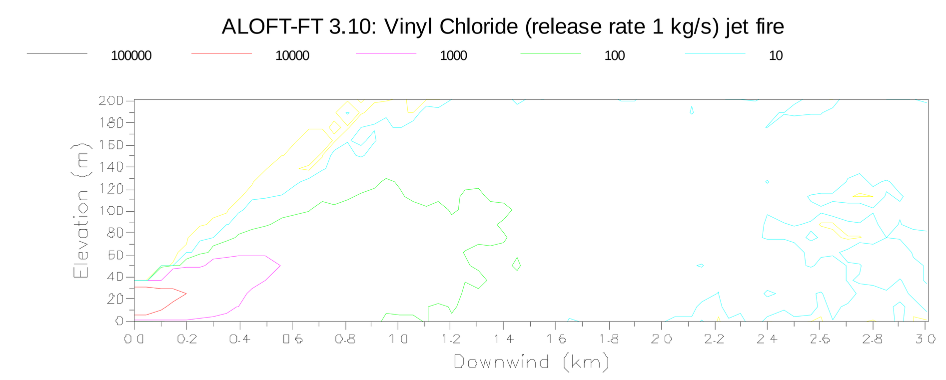
For liquid pool fires, fuel properties (heat of combustion, mass burning rate and radiative fraction) and pool surface area are required in order to determine the source term of toxic species and buoyant force. For gaseous fuels, release rate (in kg/s) needs to be estimated, e.g. according to [1].



Atmospheric dispersion of smoke plume was subsequently modelled by the ALOFT-FT [2] tool (large-eddy simulation) for the given accidental scenario (type of fire, wind speed, etc.):



Hydrogen Chloride Concentration (microgram/m3 - one hr avg) Horizontal Plane, 0 m Elevation



Hydrogen Chloride Concentration (microgram/m3 - one hr avg) Vertical Plane, 0 m Crosswind

Reference threshold (I and II) values for toxicity of individual combustion products were determined following the methodology for selection of acute exposure limits [3].

Publisher	Reference treshold I	Reference treshold II
EU	AETL- 3a AETL-3b	AETL-2
United States Environmental Protection Agency	AEGL-3	AEGL-2
Ministère de l'Écologie, de l'Energie, du Développement durable et de la Mer	SPEL	SEI
The American Industrial Hygiene Association	ERPG-3	ERPG-2
Subcommittee on Consequence Assessment and Protective Actions	TEEL-3	TEEL-2

For the multi-component mixture of toxic gases the concept of fractional effective dose (FED) [4] can be used.

CONCLUSION:

Simplified approach for estimating the emission factors from outdoor fires of dangerous chemicals, utilizable for major accident prevention and preparedness, was developed and the case study illustrating the application of the proposed method was performed. ALOFT-FT software tool based on large eddy simulation of buoyant fire plumes was employed for predicting the local toxic contamination in the down-wind vicinity of the fire. The database of model input parameters can be effectively modified enabling the simulation of the smoke plume from pool fires or jet fires of arbitrary flammable (or combustible) gas, liquid or solid.

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