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Dimensionless Analysis of Heat, Momentum and Mass Transfer in a Pool Fire

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Statistical analysis about major accidents indicate that pool fires are among the most frequently encountered major accidents in the Chemical Industry, cause the highest material and economical losses. The CFD simulation has become an important research tool in this type of fires. Also hydrocarbons are first materials to be ignited the first, in this paper, the phenomenon denominated as hydrocarbon pool fire is studied. The hydrodynamics behavior considering the turbulent flow in transient regime were coupled with mass and heat transfer transport including a generation of mas and energy due to a combustion reaction, where the chemical kinetics considering the heptane as a surrogate compound for gasoline. The results are validated comparing them with previously published experimental data, and show the presence of gradients of concentration, temperature as well as velocity. In this type of scenarios, there are numerous dimensionless numbers which can be used to describe the phenomena. These dimensionless groups provide the advantage of being able to compare behaviors at different scales, where space and time variations are generally present. As a result these dimensionless groups can be used in scaling analysis procedures.

1. Introduction

According to several statistical studies, pool fires represent a significant portion of major industrial accidents (Casal, 2008). The Figure 1 present the problem denominated as hydrocarbon pool fire, the vast complexity in these types of phenomena resides in hundreds of elemental chemical reactions with intermediate processes that involve in a great number of chemical species simultaneously (Basevich, 2013). This type of study also requires inclusion of momentum, mass and energy balances, and kinetically-influenced chemical reaction, each one with wide range fluctuations of length scales (time and space). The flow might contain eddies down to 10 –100 μm size and micro-timescale (Argyropoulos and Markatos, 2008). Thus, the prediction of the behavior of these accidents is still being subject to numerous studies, and nowadays, computer simulation has become one of the most important tools in search of feasible solutions (Vasanth et al., 2014). Particularly the CFD model is effective to analyze some complicated accident scenarios that SFM (solid flame model), is not capable of estimate (Sun et al., 2014) and useful to develop analysis of complex phenomena, which are very hard to address experimentally (Raynal, 2015).

Pool fires had been widely studied during last few decades using different approaches, experimentally (Mudan, 1984) or by computational simulation (Mishra, 2010). Although many of the studies mentioned above are focused on a single aspect of the whole problem, some others tried to couple them by studying several aspects of the phenomenon simultaneously (Faghri and Sunden, 2008). In this kind of research, both experimental and theoretical studies are important; a better understanding of pool fires can be achieved only through combining both approaches. Nevertheless, a complete pool fire predictive model that is applicable for different pool sizes in an effective way has not been developed yet (Argyropoulos, 2015). The evident complexity and variability inherent to pool fires are the principal factors for this poor development. Likewise, the lack of experimental data for large pool sizes makes the theoretical models harder to validate (Skarsbo,

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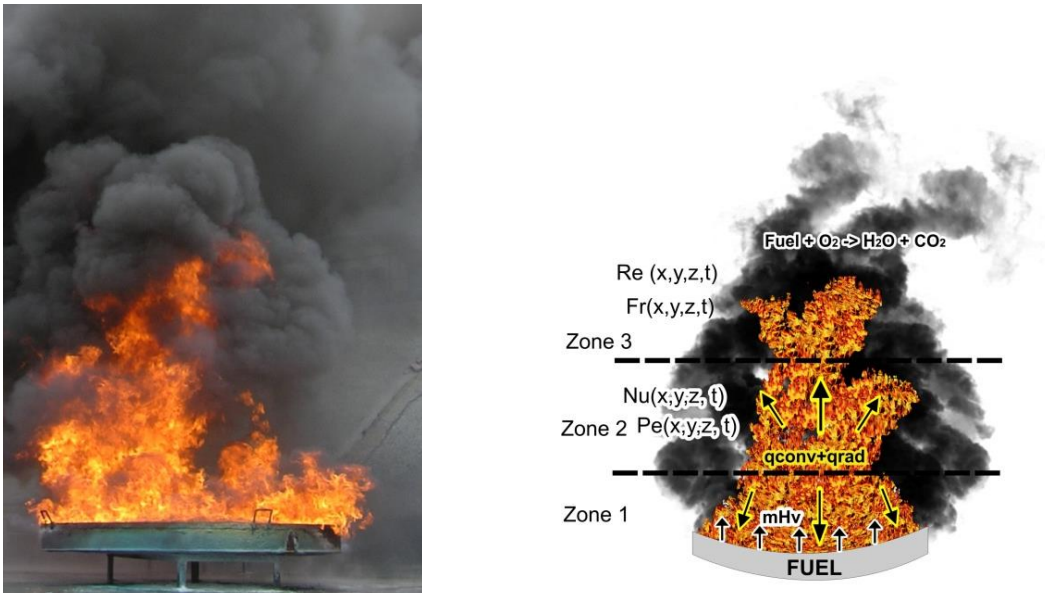
2011). Argyropoulos (2015) analyzes the literature of turbulent flows and notes that still has major failures in the models of turbulent flows, it are still common for many applications particularly those that involve strong curvature, intermittency, strong buoyancy influences, low-Reynolds-number effects, rapid compression or expansion, strong swirl, and kinetically-influenced chemical reaction. While Raynal (2015) present an overview of the simulation approaches and says it is frequently that mass and heat transfer and also chemical reactions are not taken into account. This should be the main objective for the next decade to come.



(a) Experimental fire *(b) Representation of the phenomena*

Figure 1: Hydrocarbon pool fire whit a circular geometry

In this work was implemented a CFD simulation that consider simultaneously a momentum, mass and energy transport balances, and including the combustion reaction and heat generation by reaction. This is an important characterise of this model because in CFD and simulation literature the heat generation is usually a constant volumetric term without the considering of activation energies and other important kinetic constants. The control volume (CV) approach for a pool fire is used to develop a valid model and obtain velocity, concentration and temperature profiles, which are used for get dimensionless groups, such as Reynolds and , Froude. Variables and dimensionless numbers, help to describe the characteristic behaviour of the flames (geometry, energy transport, kinetic, composition).

2. Methodology

The approach of this paper is to simulate the different phenomena in the combustion zone. Coupled momentum, mass and heat transfer equations are used for the CFD model. The momentum transfer is simulated using the turbulent flow interface k - ϵ, while the mass transfer model includes the combustion reaction of representative mixtures which have been proposed as surrogate for both gasoline and diesel (Battin-Leclerc, 2008), considering a complete conversion and applying the combustion stoichiometry proposed by Maron (1955). Also, the reaction rates and kinetic parameters given by Naidja (2002) are included in the simulation. The effect of temperature has been considered over several transport parameters and thermo physical constants, using AspenTech V 7.3 as well as MATLAB 7.8.
A selection of the kinetic parameters and properties used in this work are shown in Table 1 and Table 2 (thermodynamic properties, transport coefficients, kinetic parameters).The reaction stoichiometry used for the combustion is shown below.

2.1 Kinetic model

The fuel selected for this study was Heptane as a gasoline surrogate fuel, which follow the following reaction stoichiometry:

$$Fuel + \nu_{O_2} O_2 \rightarrow \nu_{CO_2} CO_2 + \nu_{H_2O} H_2O \quad (1)$$

The stoichiometry coefficients for heptane combustion are ν_{O_2} = -11, ν_{CO_2} = 7 and ν_{H_2O} = 8 respectively. The kinetic rate used in this work, is a modified version of single step Westbrook's kinetics (Westbrook, 1984) and showed in Eq(2).

$$r_{overal} = AT^n \exp\left(-E_a/RT\right)\left[Fuel\right]^a\left[Oxider\right]^b \tag{2}$$

Table 1: Kinetic parameters for Heptane combustion

Parameter	
A	5.1×10^{11}
E_a [kcal/mol]	30
a	0.25
b	1.5

Table 2: Thermophysical and transport properties

Property	value	Property	value
$-\Delta H_{rxn}^{488.15K}$	$449,661.52\ \left[J/mol\right]$	$D_{fuel,mix}$	$7.297\times10^{6}\left[m^2/s\right]$
Cp_{hm}^{fuel}	$25.51\ \left[J/(mol\ K)\right]$	$D_{O_2,mix}$	$2.202\times10^{-5}\left[m^2/s\right]$
$C_{O_2}^0$	$8.58\ \left[mol/m^3\right]$	$D_{CO_2,mix}$	$1.677\times10^{-5}\left[m^2/s\right]$
C_{fuel}^0	$12.96\ \left[mol/m^3\right]$	$D_{H_2O,mix}$	$2.403\times10^{-5}\left[m^2/s\right]$
$V_{O_2}^0$	$9\ \left[m/s\right]$	k_{mix}	$1.181\ \left[W/(m\,K)\right]$
V_{fuel}^0	$0.316\ \left[m/s\right]$	ρ_{mix}	$3.233\ \left[kg/m^3\right]$
G_{vap}^{fuel}	$0.4104\ \left[kg/(m^2 s)\right]$	Cp_{mix}	$1,183.71\ \left[J/(kg\ K)\right]$
$\dot{m}_{fuel}^0$	$0.725\ \left[kg/s\right]$	α_0	$3.43\times10^{-3}\left[K^{-1}\right]$
$\dot{Q}_{fuel}^0$	$0.602\ \left[m^3/s\right]$		

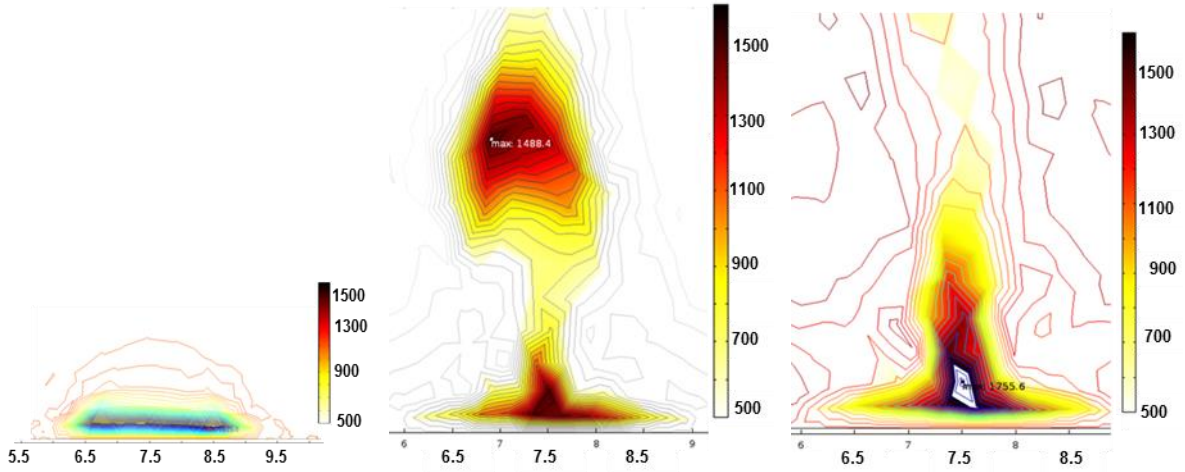
2.2 Transport models

The CFD model is constituted by continuity, momentum, RANS turbulence model, mass and energy transport equations. The respective equations are coupled and solved, considering that the phenomena occur simultaneously. The mass transport model is using diffusion – convection whit generation by reaction on transient mode for the *i* - species, where $D_{i,M}$ is the diffusivity coefficient of *i* – specie on the reacting mixture and is showed in Table 2. In the energy case, the generation is given by:

$$Q_{gen} = -\Delta H_{rxn} r_{Fuel} \tag{3}$$

3. Results and discussion

The results from CFD simulation in transient regime are presented in the Figure 2 to Figure 7. The temperature values found fluctuated between 600 and 1,500 K with some maximum local values reaching 1,500 and 1,700 K. Generally, it was observed that the maximum temperature values of the flame are located at the bottom (between 10 and 50 % of the total flame height), these results are very similar to reported in literature (Chatris, 2001) and the behaviour register by Muñoz (2004). Figure 2 show the evolution in three different instants whit geometries very different.



(a) t = 0.58 s, Tmax = 1,125K *(b) t =1.6 s, Tmax = 1,488K* *(c) t = 2 s, Tmax = 1,756K*

Figure 2: Behaviour of the geometry and temperature profile in transient regime

In Figure 3 are presented in function of time the maximum temperatures encountered in different positions in the combustion zone, and average temperatures of the simulated field, so this average temperature is a temperature lower than located in the flames region. Therefore, it can be said that flame temperatures are between these limits in the indicated instants.

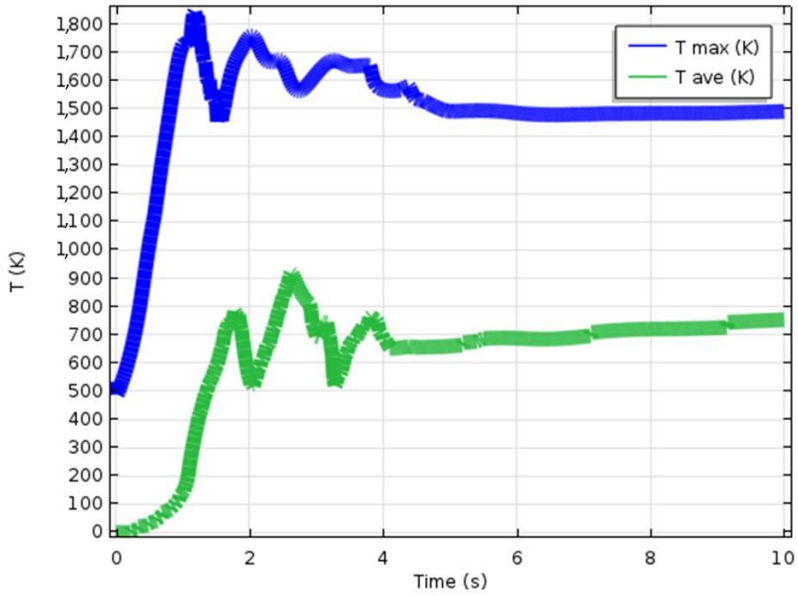
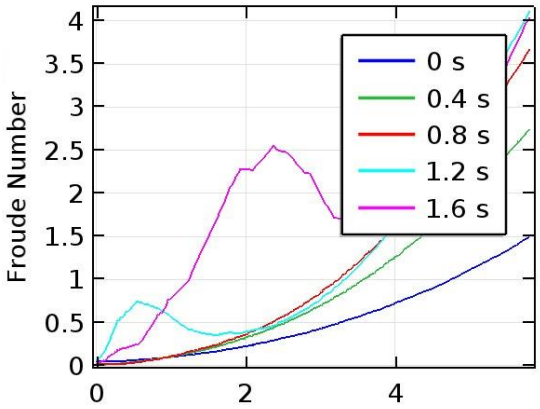
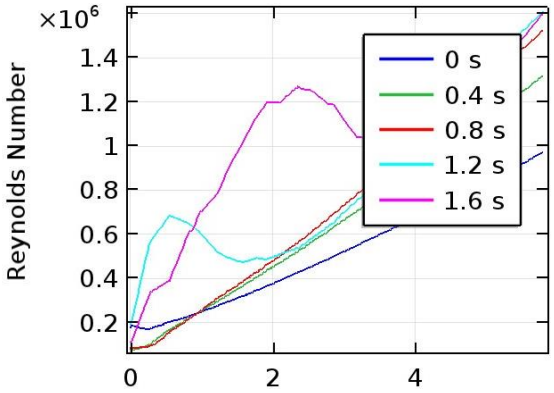


Figure 3: Maximum temperatures and average temperatures across the simulated field

In the Figures 4(a) and 4(b) the behavior of Reynolds and Froude numbers are shown, respectively. In these figures, a sharp increase is observed with Reynolds and Froude numbers at an elevation between 2.5 and 3.0 m, over the curve of 1.6 s. This deflection point corresponds in Figure 2(b), exactly where the maximum temperature is observed. This can also be seen in Figure 5, where the temperature distribution is presented in dimensionless form along the central axis. Noticed that at that moment (t = 1.6 s) other local maximum occurs in the region located near the base (0.5 m approx.). The Figure 6 displays the reaction rate of the fuel in mol/m^{3}s, t = 1.6 s after the combustion started. This confirms the existence of combustion in the central region with approximate height of 3 m because the reaction rate becomes a value different from zero. The values found for the Reynolds number clearly show that the regime is highly turbulent, while the number value of less than unit for Froude number indicates the importance of buoyancy forces.



(a) Froude number (-) in the time 0 – 1.6 s



(b) Reynolds number (-) between 0 to 1.6 s.

Figure 4: Dimensionless number along x=7.5 m, $0 \leq y \leq 6$ *m.*

Figure 7 shows the reaction rate and the Froude number on the central axis of the Pool, plotting only up to 1 m in height, this was done so to show that at the height of 0.45 m, coincided maximum temperature value (t = 2, 2.5, 3, 3.5, 4, 4.5 and 5 seconds with maximum values of temperature in K 1,756, 1,660, 1,623, 1,651, 1,567, 1,534, 1,491, respectively) an inflection is observed, although it also notes that are not maximum values Fr, Re or Reaction rate. As shown in Figures displayed, the maximum temperatures do not coincide with the maximum values of the dimensionless numbers or the reaction rate, however if inflections occur, it suggests that the conditions to find the maximum values is a very complex phenomenon It depends on many variables and non-linear behavior.

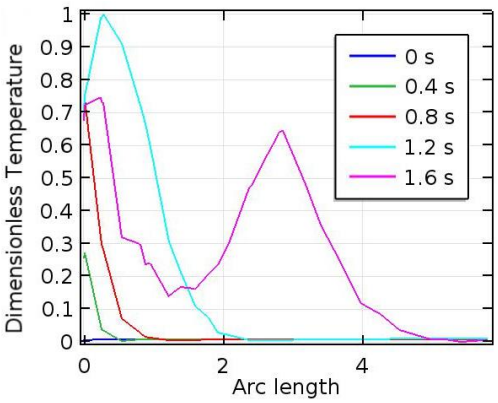


Figure 5. Dimensionless temperature along the central axis in a pool fire.

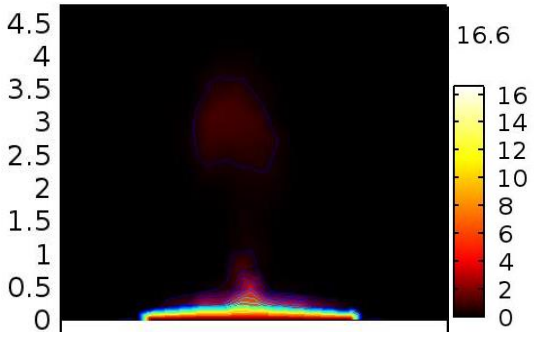
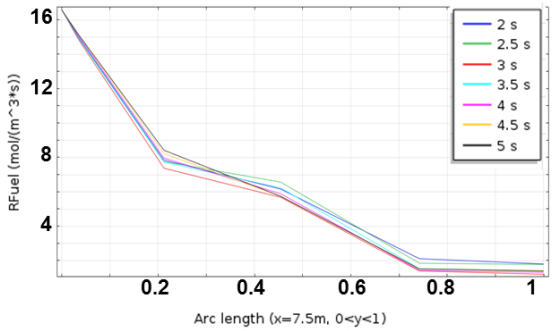
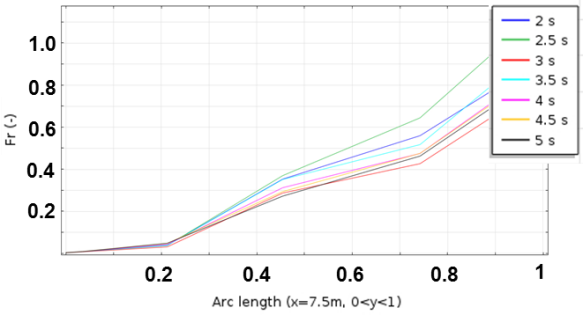


Figure 6. Reaction rate of combustion of a hydrocarbon at time 1.6 s.



(a) Reaction rate of combustion of a hydrocarbon



(b) Froude number in a pool fire.

Figure 7: Reaction rate and Froude number in the time $0 \leq t \leq 5$ *s in the combustion of hydrocarbon pool fire*

4. Conclusions

The transient behaviour of a pool fire is approach by CFD, coupling models of mass, momentum and energy. Present behaviours very similar to show in specialized literature with experimental data. The region of the flames show fluctuations between 600 to 1,500K, while maximum temperatures values are present in regions close to the base and below half the height of the flames, values between 1,500 to 1,700 K.

The selected kinetics is essential to obtain approximations of the temperature distribution, so the assumption of a global and representative reaction is a simplification which translates into cost deviations from the exact values in a fire. However it provides simulated data across the region, which comes closest to the actual behaviour of a fire.

The dimensionless numbers, by definition, are valid regardless of the scales and thus are applicable in large-scale fires and not only in pool fires of experimental sizes. The values of the Reynolds number are less than 1×10^5 in the low area, and for the temperatures maxims are $1 \times 10^5 \leq Re \leq 5 \times 10^5$, these values of turbulence are cause that flames are strongly distorted. The Froude number show small values in the region near to surface area ($Fr \leq 1$) and increases with the flame height, where the forces of momentum are dominant.

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