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CFD-Simulation großer Poolfeuer

(CFD simulation of large pool fires)

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1. Introduction

Accidental fire in process plants, e.g. pool or tank fires [1,2] show a potential risk for humans and neighboring facilities due to their thermal radiation, and formation of combustion products such as soot particles. Such fires are relatively little investigated experimentally [3-5] and especially with CFD simulations [5-7]. Detailed investigation of such fires must be done especially in a field of thermal radiation from the fire to the surrounding. CFD simulations of large pool fires are done, also to reduce the number of large scale experiments. CFD simulation offers spatially and temporally resolution of thermal radiation inside and outside the fire as a function of the fire dynamics.

In this work 3D transient CFD simulations of sooty, large, hydrocarbon pool fires e.g. JP-4 with d = 2 m, 8 m, 16 m, 20 m and 25 m are done to predict the emission temperatures (T), the surface emissive power (SEP) and the irradiances ($E(\Delta y/d)$). The large JP-4 pool fires with d = 2 m, 20 m and 25 m are also investigated by CFD under the influence of the cross wind with various wind condition ($0.7\ m/s \leq u_w \leq 16\ m/s$) to predict the influence of flame tilt and drag on the SEP_{CFD} and E_{CFD} ($\Delta y/d$). The simulations are done by using ANSYS CFX and ANSYS FLUENT softwares. Different models have been tested to find the best prediction of the experimental data.

2. Methods

2.1 Experiments

The flame emission temperatures and Surface Emissive Power (SEP) were measured by IR thermography system. For the measurements of irradiance wide angle radiometers were positioned depending on the expected heat radiation in certain intervals of the flame. To study the dynamics of large pool of flames and the determination of temperature and emitted thermal radiation the large scale experiments have been done on pool fires with different fuels and circular pool diameters of 2 m, 8 m, 16 m and 25 m [3,4].

For CFD simulation of the thermal radiation and the soot formation in a large JP-4 pool experimental data used for validation of CFD simulation are:

a) Frequency of organized structures in the fire such are hot spots and soot parcels, obtained by recording the visible range of the fire with video camera,

b) Thermograms obtained by thermographic measurements,

c) Mean irradiances $\overline{E}(\Delta y/d)$ at different horizontal distances Δy from the fire obtained by radiometer measurements.

2.2 CFD simulation

The software packages ANSYS CFX-12 and ANSYS FLUENT-12 are used with different submodels:

- Scale Adaptive Simulation (SAS) and Large Eddy Simulation (LES),
- Flamelet model with probability density function (PDF) for non-premixed combustion (800 chemical reactions and 112 species) and PDF Transport model (40 chemical reactions and 20 species)
- Lindstedt and Tesner soot model,
- Monte Carlo radiation model (MCM) and Discrete Ordinate radiation model (DOM).

The fine meshes of a fire domain with about 1 million cells are used in the simulations (Fig. 1). The cylindrical geometry is used to simulate fire in a calm condition and a rectangular geometry is chosen to predict the flame tilt under the wind influence. In a wind condition an air flow with a certain velocity which refers to the wind speed is assigned at that inlet boundary.

3. Results and discussions

SEP(fuel, d, t) is predicted by CFD simulation as an incoming radiation from inside the flame to a defined flame surface (e.g. isosurface of a constant flame temperature) [5-9]. The results obtained by CFD simulation are validated with experimental data e.g. IR-thermographic measurements of JP-4 pool fire (d = 2 m, 8 m, 16 m and 25 m) and measurements by radiometers [3,4].

From CFD predicted instantaneous temperature fields (Fig. 1, left) vertical temperature profiles $\overline{T}_{CFD}(x/d)$ for different relative radial distances y/d = 0, y/d = 0.05 and y/d = 0.1 show that the absolute maximum flame temperatures $\overline{T}_{max,CFD}(d)$ are away (y/d = 0.05) from the flame axis and depend on d: 1300 K (d = 2 m), 1250 K (d = 8 m), 1230 K (d = 16 m), 1200 K (d = 25 m) which agree well with the measured temperatures $\overline{T}_{max,exp}(d)$ [3,4].

The CFD simulation of the SEP requires a definition of the flame surface. SEP_{CFD} is predicted by using three different ways [8,9]. In the first way the flame surface is determined by using an isosurface at a constant temperature (Fig. 1). In the second way the flame surface resulted from the integration of many parallel two-dimensional distributions of incident radiation G(x,y) along the z-axis perpendicular to the xy-plane. In the third way two virtual wide-angle radiometers are defined at the both sides of the pool rim and the irradiance E(Δy/d) is simulated as a function of Δy/d.

To simulate the SEP, more exactly, a temperature dependent effective absorption coefficient $\hat{æ}_{eff}$ (T) of the dissipative structures (reaction zones, hot spots and soot parcels) and air as a four-step discontinuity function is developed [8,9].

CFD predicted $\overline{SEP}_{CFD}(d)$ values of JP-4 pool fires, obtained by the virtual radiometers are: 105 kW/m^2 (d = 2 m), 65 kW/m^2 (d = 8 m), 45 kW/m^2 (d = 16 m) and 35 kW/m^2 (d = 25 m) (Fig. 2). The SEP_{CFD} value for d = 2 m under predicts the SEP_{exp} by a factor of 0.8

whereas a good agreement is found between $\overline{SEP}_{CFD}$(d) and $\overline{SEP}_{exp}$(d) for d = 8 m, 16 m and 25 m. Based on the first way the CFD_{SEP} values agree well with the measured SEP_{exp} values if the flame surface temperature of 1100 K is used for d = 2 m, 500 K for d = 8 m and 400 K for d = 16 m and 25 m [8,9].

CFD predicted time averaged irradiances $\overline{E}_{CFD}(\Delta y/d, d)$ under predicts the measured $\overline{E}_{exp}(\Delta y/d)$ at the pool rim $\Delta y/d = 0$ for d = 2 m by a factor of 0.8 and over predicts $\overline{E}_{exp}(\Delta y/d)$ up to the factor of 1.6 at $\Delta y/d = 0.5$ whereas for d = 8 m, 16 m and 25 m the irradiances CFD E ($\Delta y/d$) agree well with the measured $\overline{E}_{exp}(\Delta y/d)$ (Fig. 3).

The CFD results predict also $\overline{T}$(d), $\overline{SEP}$(d) and $\overline{E}(\Delta y/d)$ under the influence of the cross wind (u_w = 2 m/s, 3m/s and 4.5 m/s) [9]. CFD simulations show that the wind influences the flame length, flame tilt, flame drag, the flame temperatures T, the SEP and the irradiances E [9]. With increasing wind velocity u_w from 4.5 m/s to 10 m/s $\overline{SEP}_{CFD}$ and $\overline{E}_{CFD}$ ($\Delta y/d$) at the pool rim increase downwind by a factor of about 2 – 6 for d = 2 m and by a factor of about 2 – 7 for d = 20 m and 25 m. In both cases $\overline{E}_{CFD}(\Delta y/d)$ do not increase if $u_w > 10$ m/s as it is found in experiments [9]. In the upper section of the flames, depending on the flame tilt and drag, a decrease of flame temperature of several hundred K is found.

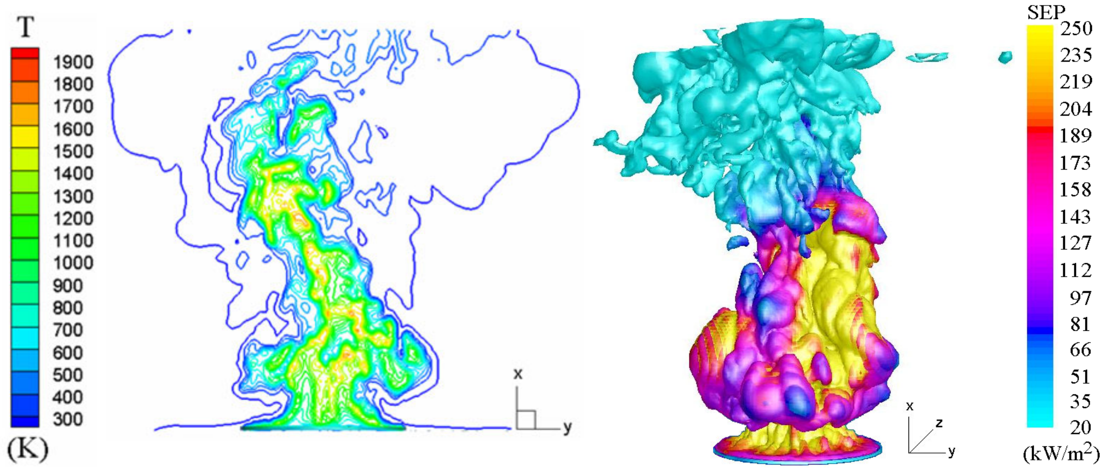

Fig. 1: Instantaneous isotherms (left) and isosurface at T = 400 K superimposed with SEP (right) of JP-4 pool fire (d = 16 m).

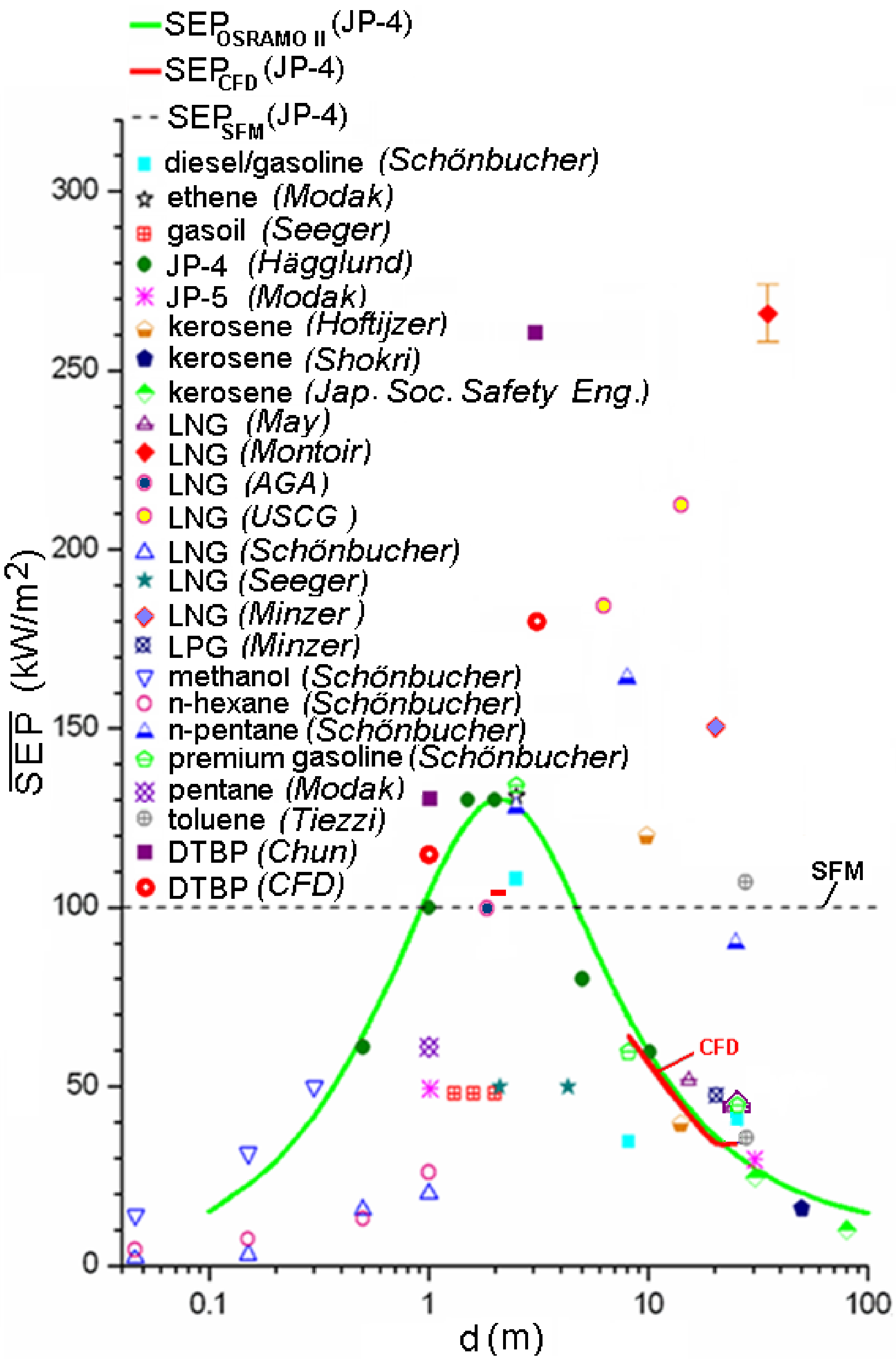

Fig. 2: Measured and CFD predicted $\overline{\mathrm{SEP}}$ of hydrocarbons and DTBP pool fires as a function of d.

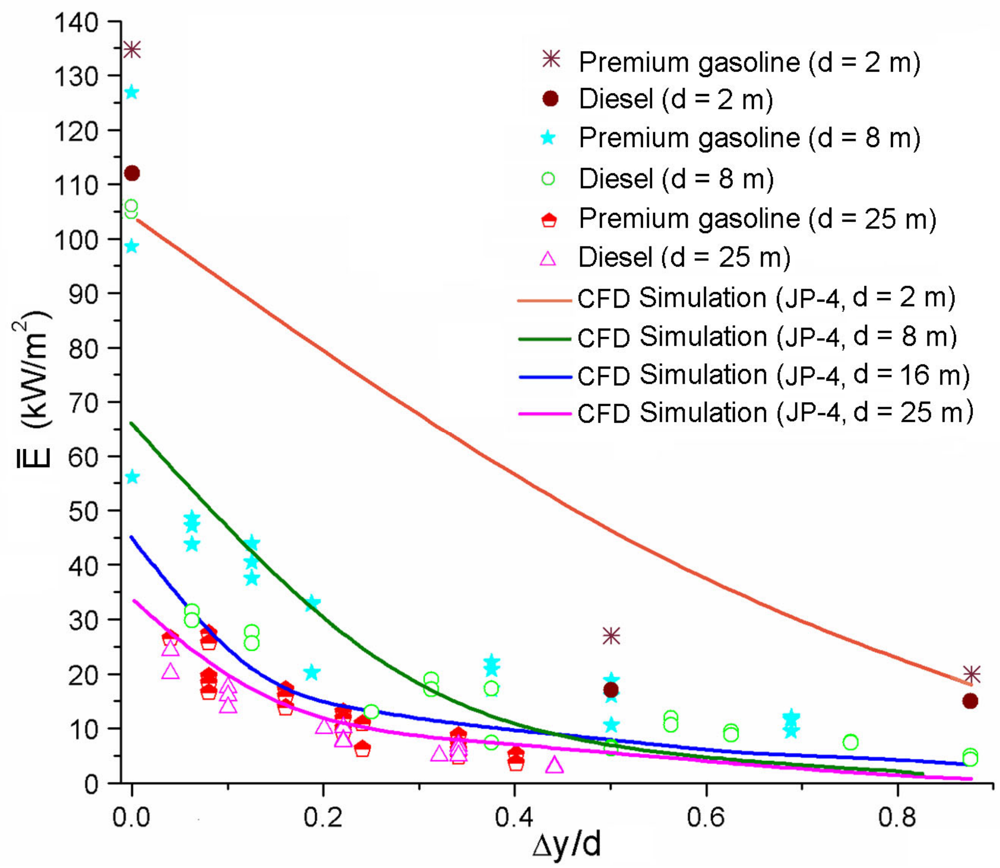

Fig. 3: Measured $\overline{E}_{exp}(\Delta y/d)$ and CFD predicted time averaged irradiances $\overline{E}_{CFD}(\Delta y/d)$ from the large JP-4 pool fires as a function of relative distance $\Delta y/d$ from the pool rim.

4. Conclusion and outlook

With the proposed CFD simulation it is possible to improve the assessment of the potential hazards in the plants of the processing industries caused by sooty hydrocarbon fires. This is important to include the new method in regulation and implementation of safety analysis reports, emergency response planning and quantitative risk assessment (QRA). CFD simulation can predict safety distances between a plant and the surroundings (people, buildings, environment).

CFD based modeling of fires can be successfully used to reduce expensive experimental work on large scale pool fire investigations.

The CFD simulations allow (for future), the estimation of an influence of multiple fires on the hazard potential.

The future CFD simulations will include more hydrocarbon fuel pool fires (methane, n-pentane, n-heptane, kerosene, LNG) with different pool diameters ($1\ \mathrm{m} \leq d \leq 25\ \mathrm{m}$) to investigate SEP(fuel, d, t), E(fuel, d, t) and soot mass fraction from the fires.

Various mean absorption coefficients will be used to investigate their influence on the $\overline{SEP}(d)$ and $\overline{E}(\Delta y/d)$ from the fires.

Different submodels and their combination will be used to study their influence on the CFD predicted $\overline{SEP}(d)$, $\overline{E}(\Delta y/d)$ and soot mass fraction of the fires. A special attention will be paid on the influence of chemical reactions (e.g. flamelet models) on the results.

References

[1] M. Hailwood, M. Gawlowski, B. Schalau, A. Schönbucher, Chem. Eng. Tech. 32 (2009) 207

[2] The Buncefield Investigation, Progress Report, February 2006, www.buncefieldinvestigation.gov.uk/report.pdf.

[3] D. Göck, Experimentell fundierte Ballenstrahlungsmodelle zur Bestimmung von Sicherheitsabständen bei großen Poolflammen flüssiger Kohlenwasserstoffe, Dissertation, Universität Stuttgart, 1988.

[4] R. Fiala, D. Göck, X. Zhang, A. Schönbucher, Chem. Ing. Tech. 63 (1991) 760 – 761.

[5] H. Chun, I. Vela, K.-D. Wehrstedt, A. Schönbucher, Thermal radiation of di- tertbutyl peroxide pool fires – experimental investigation and CFD simulation, J. Hazard. Mater. 167, 1-3 (2009) 105-113

[6] I. Vela, C. Kuhr, A. Schönbucher, CFD-Modeling of Large-Scale Kerosene Pool Fires; Proceeding of the 11th International Symposium on Loss Prevention and Safety

Promotion in the Process Industry - Loss Prevention 2004, ISBN 80-02- 01574-6, 3143–3147
[7] M. Gawlowski, M. Hailwood, I. Vela, A. Schönbucher, Deterministic and probabilistic estimation of acceptable separation distances – consequences for industrial sites, Chem. Eng. Technol. 32 (2009) 182–198
[8] I. Vela, H. Chun, M. Gawlowski, K.B. Mishra, M. Rudolph, P. Sudhoff, K.-D. Wehrstedt, A. Schönbucher, Vorhersage der thermischen Strahlung großer Kohlenwasserstoff - und Peroxid- Poolfeuer mit CFD Simulation, Forsch. Ingenieurwes. 73, 2 (2009) 87-97
[9] I. Vela, CFD prediction of thermal radiation of large, sooty, hydrocarbon pool fires, Dissertation, Universität Duisburg-Essen, 2009.