CFD ANALYSIS OF MIXING AND RESIDENCE TIME DISTRIBUTION IN COOL FLAME VAPORIZERS

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Abstract. In this paper the fluid dynamics of three cool flame vaporizers are investigated numerically, using a commercial CFD-code. The paper focuses on analyzing local and global residence time distributions (RTD). Two approaches have been used to model the RTD: a transient step tracer model (which serves as a reference) and a dispersed phase tracer model.

1 INTRODUCTION

Mixture preparation is one of the essential processes for efficient use of liquid fuels in combustion and reforming technology. A promising way enhancing the process of vaporization of hydrocarbon spray is provided by making use of the cool flame phenomenon. Cool flames are exothermal reactions occurring in mixtures of certain hydrocarbons with air at temperatures between 250 °C and 500 °C.

Stabilized cool flame reactors for vaporizing liquid fuels may be regarded as mixing devices. The fuel spray is injected into the reactor where it is evaporated. The heat needed for vaporization is partially provided by the cool flame reaction, which stabilizes in discrete regions of the reactor.

The amount of heat released per unit volume by the cool flame reaction is low compared to the amount of heat per unit volume needed for vaporization of the fuel spray. Therefore the process constitutes a thermo chemical system which may react very sensitive on inappropriate heat and mass transfer inside the reactor. The transport of heat into the region of spray vaporization occurs via recirculation flow. Here two types of recirculation flow may be distinguished: recirculation induced by a confined jet or recirculation around a flame tube both of which are regarded in this paper.

Implementing cool flames in technical apparatus reveals challenges concerning reaction stability and macro mixing. Mixing energy is delivered by the momentum of the inlet air flux. Therefore air and fuel inlet need to be arranged appropriately to ensure for appropriate mass and energy transport. Furthermore cool flame reactors are often implementing a start burner which is needed to heat the system to operating temperature. To guarantee flame stabilization the reactor needs to have an appropriate design.

The residence time distribution (RTD) is a very important characteristic to judge for
mixing and flow inside the reactor, particularly about the nature of the recirculation flows. To analyze the RTD of existing reactors and to prepare for experiments, CFD analysis has been performed.

2 NUMERICAL ANALYSIS OF FLOW AND RESIDENCE TIMES

In recent years different reactor geometries have been developed and successfully implemented. It was shown by Hartmann\(^1\), that reactors of similar volume show individual behavior regarding their stability limits.

In figure 1 two geometries are shown. In the multi jet reactor on the left the air nozzles are arranged around the fuel nozzle, which is located on the reactor axis. The reactor is equipped with a recirculation tube and a deflector plate. The reactor on the right implements a single jet loop reactor geometry. A third reactor has been analysed, which has the same design as the single jet reactor, but misses the recirculation tube. All three reactors are designed to operate at similar power ranges and have proved good operability in technical application\(^1\).

![Figure 1: Cool Flame reactor designs: multi jet (left), single jet (right)](image)

The flow was modelled using the commercial software ANSYS CFX. To account for turbulence the k-\(\varepsilon\) model was chosen. The fuel was modelled using a Lagrangian tracking approach. Heat and mass transfer was accounted for with the well known model of Ranz- and Marshall\(^2\).
The total view of the flow for two reactors is shown in figure 1. For the multi jet system (left) large vortex areas are shown at the inner walls of the recirculation tube and behind the deflector plate, which acts like a bluff body. For the single jet system (right) large vortices are observed at the outlet of the flame tube. Vortices are representing areas of locally higher residence times. It was observed experimentally, that cool flames are stabilized mainly in zones of higher residence times which are the areas in the vortex zones and around the recirculation tubes.

Modeling of mass transfer in the large vortex regions is limited since RANS-turbulence modelling was chosen here which transfers macro mixing effects (turbulent transport in small eddies) into a micro mixing process (gradient diffusion). However, the recirculation flow through the gap around the recirculation tube may be imagined as bulk flow and so macro mixing characteristics, such as recirculation frequency around the tube, should be possible to be observed experimentally and numerically via investigation of the residence time distribution at the outlet.

To determine RTD at the outlet, two different methods have been used. The first one resembles the step tracer experiment which is a standard procedure to determine residence times. Based on a converged steady state solution a transient simulation for a tracer variable is performed, which is generated by a step boundary condition at the inlet at time zero of the transient run. The response at the outlet boundary condition is monitored and is interpreted in its dimensionless and normalized form as the residence time distribution function \( F(\theta) \) from which the residence time density function \( E(\theta) \) may be derived:

\[
E(\theta) = \tau \frac{dF(\theta)}{dt}
\]

where \( \tau \) is the mean (hydraulic) residence time and \( \theta = t/\tau \) is the dimensionless time.

As an alternative and computationally cheaper method Lagrangian Particle tracking was used. The residence time distribution density is achieved by regarding the particles as tracers which are travelling through the reactor via characteristic flow paths. The residence time for each particle is obtained by integrating over particle velocity and travelling distance.

Based on the steady state flow field particles were tracked through the flow field according to the equation

\[
m_p \frac{dv}{dt} = \frac{1}{8} \pi \rho_l d^2 C_D \left| v_i - v_p \right| \left( v_i - v_p \right)
\]

The equation was solved by a forward Euler method. For the calculation of the drag coefficient \( C_D \) the Schiller-Naumann drag model has been used. To account for turbulent dispersion of the dispersed phase, a model based on the work of Gosman and Ioannides\(^3\) is used, which calculates the macroscopic transport of droplets by turbulent flow structures. The dispersed Phase is introduced to the flow at the inlet boundary condition. The number of events has been varied from \( 0.2 \times 10^5 \) to \( 1 \times 10^5 \).
3 RESULTS AND DISCUSSION

In figure 2 the residence time density function $E(\theta)$ determined by the transient tracer model, which may be treated as the reference, is compared to the residence time density distribution determined with the dispersed phase tracer model for the multi jet reactor is shown. The results are compared to an ideally continuously stirred tank reactor (CSTR). Both curves are showing a set of consecutive peaks. The first peak which represents the shortcut path through the reactor is followed by maxima of decreasing intensity, which are representing loops of the tracer around the recirculation tube. In figure 3 characteristic paths for the first two peaks are shown. For growing $\theta$ the transient simulation is approaching to the behaviour of the CSTR since the transient effect of the recirculation around the flame tube disappears and only diffusive tracer transport dominant. As can be seen at the $F(\theta)$ curves, short residence times of the tracer were determined for the simulations with the dispersed phase. Since the particles paths are determined by macro mixing effects (bulk flow and turbulence dispersion model) transport velocity is of the order of the local velocity. The high gradients between the peaks, shows, that the effect of micro mixing (gradient diffusion) is not considered. Furthermore it seems that the transport of particles via the turbulent shear layer is underestimated by the turbulent dispersion model.

![Graph showing residence time distribution and residence time density distributions for the step tracer model and for the transient phase model](image-url)
A significant part of the dispersed phase (about 20%) does not leave the reactor within the integration limits, i.e. gets trapped inside the vortex zones or the recirculation loops. Variations of the particle number have shown that the share of particles remaining inside the reactor is not a function of the number of events, which are tracked. However, the characteristics of the main flow, particularly the frequencies of recirculation, have been predicted very close to the transient case.

In figure 4 the residence time density distribution and the residence time density function of the three reactor designs are compared. For the single jet reactors a distinct shortcut flow behaviour is observed which is characterised by the first peak at small values of $\theta$. This shortcut flow is prevented in the multi jet reactor by the deflector plate. The reactors equipped with a recirculation tube show consecutive peaks with decreasing intensity, whereas the reactor without flame tube shows steady distribution of residence time density after the shortcut peak. Obviously the residence time distribution is shifted to shorter $\theta$-values when using a recirculation tube, since bulk particle transport is dominating the recirculation flow around the tube. This may be interpreted by the particles moving with the mean flow around the recirculation rather than being trapped in large vortex regions.
4 CONCLUSIONS

Residence time distributions of different cool flame reactor designs have been modeled using two approaches. The first approach follows the experimental step tracer method. Based on a converged steady state solution a transient simulation for a tracer variable is performed, which is generated by a step boundary condition at the inlet at time zero of the transient run.
As an alternative method Lagrangian Particle Tracking was used. Both approaches have shown comparable results. The dispersed phase tracer model determined shorter residence time distributions compared to the transient tracer model, which is regarded as a reference. The characteristics of the main flow, particularly the frequency of the recirculation around the flame tube, were captured by both models.

The different types of recirculation in the reactor resolve to different patterns in the residence time distribution functions. Particularly the recirculation around the flame tube leads to a stepwise increase of the distribution function is observed.

Experimental determination of residence time distribution is rather complicated for this application since the timescales, which are to be resolved are small. Modeling residence time distribution by CFD may support experimental work significantly.

REFERENCES

