MULTICOMPONENT DROPLET EVAPORATION OF HEATING OIL USING A CONTINUOUS THERMODYNAMICS MODEL

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Key words: Evaporation, Droplets, Lagrangian Tracking, Heating oil

Abstract. For the development of pre-evaporation burners, so called blue flame burners, the knowledge of the evaporation length of liquid fuels is important. In these burner systems heating oil is atomized by pressure swirl nozzles in a mixture of air and recirculated exhaust gas. Thereby, the evaporation process influences mixture preparation and the position of the flame front. Incompletely evaporated droplets could reach the flame front and increase emissions of the combustion process.

Numerical calculations are applied to the analysis of the burner and mixture preparation. Evaporation models implemented in commercial CFD codes contain many simplifications which enable their use for different applications and improved numerical stability. These models normally reduce the evaporation process to a single component and are unable to represent the distillation range of heating oil.

Within the scope of this work a film evaporation model for multicomponent fuels is implemented in a CFD code. For the determination of the composition and characteristics of the fuels pseudo components are used. The thermodynamic values of these components are control points for the continuous functions of the mixture properties. The two phase flow is modelled by an Eulerian-Lagrangian approach. The model is verified by measurements of Ochs [1]. Referring to the investigation of the evaporation process for single droplets and sprays the evaporation characteristics of heating oil droplets can be represented by the continuous thermodynamics model.

1 INTRODUCTION

Various applications for liquid fuels require a conditioning system which produces a homogenous mixture of fuel vapour and an oxidiser. Fuel cells with a catalytic partial oxidation reformer for heating oil require a separate device to evaporate the fuel oil and mix it with air. According to Hartmann [2], a cool flame reactor is a possible implementation for a conditioning system in fuel cell applications. In this appliance low temperature oxidation reactions of educts in a temperature range from 673 K - 723 K are used to provide the heat of evaporation.

In a blue flame burner, pre-conditioning of the fuel is integrated in the burner layout. Heating oil is evaporated by recirculated exhaust gas and simultaneously mixed with fresh air. The flame is stabilised downstream after this zone.

Technical fuels like fuel oil or diesel are composed of several hydrocarbons. The composition differs with the originated applied crude oil. Heating oil typically contains 40 - 70% linear and branched alkanes, 10 - 30% cyclic alkanes, 0.1 - 5% alkenes and 10 - 30% aromatics with maximum amounts of 10 % di-aromatic hydrocarbon and 3% tri- and poly-aromatic hydrocarbon. Main aliphatic components are C11 - C23 with boiling temperatures in the temperature range of 468 to 653 K. The determination of low temperature evaporation zones by numerical calculations often surrogate fuels like decane, hexadecane and Jet A-1 surrogate are applied which are not able to represent the distillation range of technical fuels. Hence in this paper an evaporation model based on the concept of continuous thermodynamics and developed by Ochs [1] is implemented into a commercial CFD code. The aim of the present paper is to validate this concept in the framework of Eulerian-Lagrangian multiphase flow single droplet modelling. Additionally, the numerical simulation of the evaporating spray is compared with the measured evaporation length and initial results of a numerical investigation of a domestic burner are presented.

2 MODELING DROPLET EVAPORATION

2.1 Film model

Referring to Ochs [1] a droplet evaporation model with the following assumptions provide adequate precision to calculate the single droplet evaporation times:

- Heat and mass transfer at the droplet can be calculated by the uniform temperature film model with a constant film thickness δ . Since the surrounding gas layer is at rest only molecular thermal conduction and diffusion can be assumed.
- No chemical reactions occur during droplet overheating. Cracking of fuel is neglected.
- The partial vapour pressure at the droplet surface is equal to the saturation vapour pressure.
- Droplets have a spherical shape.
- Heat transfer by radiation and natural convection is neglected.
- Temperature and concentration profiles are quasi-stationary.
- Properties of gaseous mixture in the film can be assumed as constant by using the reference point quantities, see figure 1.
- Internal heating is neglected.

Film model:



Figure 1: Film model with constant film thickness

Generally, the conservation equations for mass, momentum, energy and species concentrations have to be solved together with the liquid phase conservation equations. In order to evaluate heat and mass flow at the droplet surface a gaseous boundary layer around the droplet is assumed. The mass flow from fluid to gas phase caused by evaporation is derived from the law of conservation and taking into account molecular diffusion flow and assuming so called Stefan flow problem. Furthermore, the diffusive flows by pressure and temperature gradients are neglected. This leads to the following equation for the total mass flux m:

$$\dot{m}_{v} = \pi \, d \, \rho_{g,ref} \, D_{va,ref} \, Sh_{eff} \, B_{m} \tag{1}$$

with *d* the droplet diameter, ρ the density, *D* diffusion coefficient and Sh_{eff} the effective Sherwood number and B_m the Spalding mass transfer number respectively. This latter mass transfer number is defined by:

$$B_m = \frac{\xi_{\nu,s} - \xi_{\nu,\infty}}{I - \xi_{\nu,\infty}} \tag{2}$$

in which ξ is the species mass fraction at the surface and at infinity. The heat transfer from the gas towards the droplet can be described as:

$$Q_s = \pi \, d \, \lambda_{g,ref} \, Nu_{eff} \left(T_{g,\infty} - T_d \right) \tag{3}$$

with λ the heat conductivity of the gas, Nu_{eff} the effective Nusselt number and T_g and T_d the gas and droplet respectively. This equation accounts for the energy transport by thermal conduction and molecular diffusion. The heat transfer based on concentration gradients (Dufour effect) is neglected. The effective Sherwood and Nusselt numbers can be derived when assuming that the thickness of the film in the case of high evaporation rates equals the low evaporation rates (constant film thickness):

$$Sh_{eff} = Sh_0 \frac{ln(1+B_m)}{B_m}$$
(4)

$$Nu_{eff} = Nu_0 \frac{\ln(1+B_h)}{B_h}$$
⁽⁵⁾

with B_h the heat transfer number. The dimensionless number for the low evaporation rates Sh_0 and Nu_0 are modelled by the correlations from Beard et al [3]:

$$Sh / Nu = f(Re, Sc, Pr):$$

$$Re > 2: \quad 1.56 + 0.616 \cdot Re^{1/2} Sc^{1/3}$$

$$Re \le 2: \quad 2 + Re(0.435 \cdot Sc^{1/3} - 0.22)$$
(6)

2.2 Continuous thermodynamics

In contrast to a single component droplet the properties of a multicomponent droplet change with the progress of the evaporation. The concept of continuous thermodynamics purposed by Cottermann [7] takes this into account. By defining all characteristic properties in subject to the progress variable q_m , which describes the ratio of the evaporated fuel mass as given below, a multicomponent fuel can be reduced to one effective component.

$$q_{m,b}(t) = 1 - \frac{m_b}{m_{b,0}}$$
(7)

Supporting points of the continuous properties functions are modelled by Single Carbon Number (SCN) fractions [4] which are pseudo components composed of a paraffin, a naphthene and a aromatic hydrocarbon with a similar boiling point. Figure 2 shows the distillation range of a heating oil with the corresponding SCN fractions.



Figure 2: Distillation range of heating oil [1], SCN-fraction

The equilibrium molar concentration of every fuel component in gaseous phase depends on its molar concentration in the liquid phase and the vapour pressure.

However, at low temperature the high-boiling components are not relevant. Hence an active fraction, which are composed only by the relevant fractions and depends on the progress variable q_m , is defined. The boiling temperature of the active fraction is given by:

$$T_{s,akt} = T_s(q_{m,b}) \tag{8}$$

Assuming an ideal solution the molar fractions in liquid and gaseous phase are calculated by the following equations:

$$x_{akt,b,s} = \sum_{i=i_{min}}^{i_{max}} x_{i,b,s}$$
(9)

$$x_{akt,g,s} = x_{akt,b,s} p_{v,akt} \tag{10}$$

2.3 Model implementation

The multicomponent droplet evaporation model described in the previous chapter is implemented in the commercial CFD-code ANSYS® CFX 11.0 by using User Fortran Routines. The results presented in this paper are obtained by the Lagrangian tracking two-way-coupling procedure. The well known equation of Schiller Naumann is used for modelling the drag force of the droplet in the gas flow:

$$C_D = \frac{24}{Re} \left(1 + 0.15 R e^{0.687} \right) \tag{11}$$

The turbulent dispersion force based on the Favre average of the drag force is used in some calculations. To overcome difficulties with the progress variable q_m in polydisperse sprays it was necessary to implement a tracer in order to calculate the ratio of evaporated fuel mass by the increase of the tracer concentrations.

3 VALIDATION SINGLE DROPLET EVAPORATION

3.1 Settings

The vaporization behaviour of single n-octane, n-tetradecane and light heating oil droplet has been extensively investigated by Ochs [1]. The experiment consists in injection a monodisperse stream of droplets normally to a circular turbulent jet of hot air at atmospheric pressure. Two air inflow temperature conditions were investigated: T = 583 K and T = 783 K. Calculation results of the test case at an air flow temperature of T = 588 K are shown in figure 3. The temperature and velocity profile of the air jet with the trajectories of droplets with and without turbulent dispersion are visualised.



Figure 3: Test case configuration, calculation of single droplet evaporation with (right) and without turbulent dispersion (left), temperature and velocity profile, $T_{Air} = 588$ K

3.2 Results

In the first instance the computation of the gas flow is controlled by measurements. The inflow boundary conditions are set to given velocity and temperature profiles at the outlet of the heated tube. The buoyancy force was taken into account in the computations. The best agreement of measured and calculated profiles downstream is found for the turbulence model RNG-k ϵ . The results of the comparison for the air inflow temperature of T = 588 K at the position x = 312 mm are presented in figure 4 – 6. The agreement is very good for the axial velocity with a maximal relative error of 12% and fairly good in the relevant range for the vertical velocity, but at the boundary area a maximum departure of 100% is found. Since the maximum absolute error only amounts to 0.3 m/s no influence on droplet evaporation is expected.



Figure 4: Comparison of measured and calculated axial velocity profiles, air jet, T = 588 K



Figure 5: Comparison of measured and calculated velocities in z-direction, air jet, T = 588 K

Most importantly, in such hot environment the evaporation process is dominated by heat transfer. An excellent agreement is found in the temperature profiles, see figure 6, with less than 2% maximum error in the numerical computation with respect to the temperature measurements.



Figure 6: Comparison of measured and calculated temperature, air jet, T = 588 K

A similar degree of accuracy is obtained for the case with an air temperature of T = 783 K.

The computated evaporation times of single droplets with a diameter of $d = 41.9 \,\mu\text{m}$ plotted in figure 7 show that the use of the surrogate fuel hexadecane lead to shorter evaporation times. The calculation based on the continuous thermodynamics model matches very closely to the measured evaporation process. To account for the influence of the turbulence on the evaporation, a turbulent dispersion model is used. The difference to the calculation without this model is small. Since a few droplets leave the hot mainstream the average droplet diameter drops more slowly.



Figure 7: Comparison of measured and calculated droplet evaporation times of single droplets, $d = 41.9 \mu m, T = 583 K$

Figure 8 and 9 present the comparison results of further measured and calculated heating oil droplets concerning the time gradient of droplet diameter. The agreement is very good for small droplets with a diameter of $d = 41.9 \,\mu\text{m}$ and $d = 42.4 \,\mu\text{m}$ and good for the droplets with a bigger diameter of $d = 63.1 \,\mu\text{m}$ and $d = 61.9 \,\mu\text{m}$. In this case the maximum departure is 30 % with respect to the measured diameter. One possible reason is the overestimated or underestimated influence of the turbulence on the droplets by the used turbulent dispersion model. A greater variance of droplet trajectories leads to longer evaporation times because several droplets leave the hot mainstream. Without dispersion all droplets use the same path in the air stream. This results in a local heat sink and a fuel vapour source which also increase evaporation times.



Figure 8: Comparison of measured and calculated droplet evaporation times of single droplets, $d = 41.9 / 63.1 \mu m$, T = 588 K



Figure 9: Comparison of measured and calculated droplet evaporation times of single droplets, $d = 42.4 / 61.9 \mu m$, T = 783 K

4 CALCULATION SPRAY EVAPORATION

4.1 Settings

In the framework of investigations of the cool flame reaction Mengel [5] also examined the overall evaporation length and time of a spray from a pressure swirl nozzle for domestic burners. In a double wall glass reactor with a inner diameter of d = 90 mm a spray produced by a simplex solid cone nozzle 60° was evaporated in heated air, shown in figure 10. The evaporation zone was visualised by a laser sheet.



Figure 10: Test case configuration spray evaporation, laser sheet

A constant thermal fuel power of $P_{oil} = 9.5$ kW and an air ratio of $\lambda = 1.2$ were set. The nozzle pressure was 9 bar. An experimental study concerning the spray characteristics of hollow cone pressure swirl nozzle 60° performed by Lampe [6] gives start conditions for the present numerical investigation with sprays. For the examined pressure of 9 bar the interpolated and averaged values are listed in table 1.

Pressure nozzle	9 bar
Axial distance to nozzle	5 mm
Outer radius	3 mm
Inner radius	2.4 mm
Modified inner radius	1 mm
Outer angle	68°
Inner angle	62°
Modified inner angle	40°
Velocity	15.8 m/s
Averaged diameter droplet	30 µm

Table 1: Start parameter of the spray modelling

Since the nozzle used in the experiments produces a solid cone the inner angle and radius is modified to get a more realistic spray shape. The droplet distribution is approximated by Rosin-Rammler distribution with power n = 3.

4.2 Results

Figure 11 shows the result of the calculation in comparison to the experiment with an air inflow temperature of 573 K. The shape of the spray can be reproduced by the computation. The calculated overall evaporation length is 30% shorter than the experimental length.



Figure 11: Calculation spray $T_{Air} = 573$ K, $p_{Nozzel} = 9$ bar, $\lambda = 1.2$, $P_{Oil} = 9.5$ kW compared with measurement

In the cases of an air inflow temperature of T = 493 K, 613 K and 673 K the agreement is very good with a maximum departure of 15 % which is shown in figure 12. At low temperature the modelling of the spray evaporation fails. In these cases the calculation shows that the spray is not evaporated completely before it reaches the end of the reactor. As given by the simulation results at air temperature of T = 493 K with different spray angle and same droplet velocity and diameter distribution the evaporation length depends strongly on the direction of the spray inlet. Referring to the calculation with a homogenous spray distribution over the full spray angle of 60° the evaporation length is overestimated in the full temperature range.



Figure 12: Comparison of calculated and measured evaporation length of spray $T_{Air} = 453 \text{ K} - 673 \text{ K}$, $p_{Nozzle} = 9 \text{ bar}, \lambda = 1.2, P_{Oil} = 9.5 \text{ kW}$

Hence, detailed measurements of droplet trajectories and modelling are required to get a better agreement.

5 FURTHER INVESTIGATIONS: COMPUTATION OF A DOMESTIC BURNER

In the framework of a material experimental study to flame tubes in domestic burners the multicomponent droplet evaporation is applied to calculation of such a system, see figure 13. In the presented case material damages occur on the fire tube. A possible reason for these damages is the impact of droplets on the tube surface. The aim of the investigation is to determine the evaporating trajectories.



Figure 13: Domestic burner for heating oil, first simplified calculation

Since the temperature in the conditioning zone dominates the evaporation process it is important to reproduce thermal boundary conditions exactly. The temperature in the evaporation zone is influenced by the ratio and temperature of recirculated exhaust gas, the position of the combustion zone and the heat transfer by radiation and convection especially towards the surrounding heat exchanger. In figure 13 the first result of a calculation is shown. The use of an eddy dissipation concept as a combustion model leads to insufficient agreement between measured and calculated material temperatures of the flame tube. Therefore, a finite rate chemistry model will be used for this examination.

6 CONCLUSIONS

- A model for multicomponent droplet evaporation based on the concept of continuous thermodynamics was successfully implemented into the commercial CFD-code ANSYS® CFX 11.0.
- Comparable results are presented in the present paper between the numerical and experimental data for single evaporating heating oil droplets at two different air

temperatures (588 K, 783 K). Furthermore, the evaporation time and droplet diameter gradient are in satisfactory agreement.

- The comparison of experimental investigation of spray evaporation and corresponding computation shows that the overall evaporation length can be calculated for a certain temperature range. For a better accuracy further investigations with respect to the spray trajectories are necessary.
- The application of the multicomponent evaporation model for a domestic burner is in progress.

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