A MULTI-COMPONENT DROPLET EVAPORATION MODEL FOR REAL AVIATION FUELS AT ELEVATED PRESSURES

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Abstract

During the design process of modern low emission jet engines, experimental investigations of the fuel preparation process are more and more supported by numerical predictions. Using the correct properties of the specific fuel is crucial for the prediction, as the emission of advanced low emission combustors is strongly affected by the local air-fuel ratio. In this paper a novel droplet evaporation model is introduced by which the change of the thermo-physical properties of multi-component fuels during droplet heat-up and evaporation is accounted for. The model is essentially an extension of the Uniform Temperature Model [4] and, therefore, requires only slightly higher computational effort at significantly improved accuracy.

Introduction

Inherent to existing droplet evaporation models is the restriction of relying on a model fuel consisting of a few components. Since real aviation fuels are a blend of several hundred species, an evaporation model is required, which accounts for the thermo-physical properties of a multi-component fuel mixture.
The new, computational effective multi-component evaporation model, the Distillation Curve Model (DC model) is capable to reflect the distillation curve of the real multi-component fuels, like kerosene, diesel or gasoline. The major feature of the DC model is to describe the droplet evaporation process as a function of a single variable: The actual mean molar weight of the fuel inside the droplet. An additional advantage is that the model is based on analytical expressions.
The DC model is valid at elevated pressures and temperatures which are typical for technical combustion chambers. In order to take into account high pressure effects, liquid-vapor phase equilibrium has been incorporated into the model. Real gas effects are also considered within the correlations and mixing rules.
The major objective of the present paper is the adaption of the previously published DC model for multi-component aviation fuels [8] to elevated pressures. In addition, a comparison of the results predicted by the new Distillation Curve Model to the accurate Diffusion Limit Model (DL model) is presented for atmospheric and elevated pressures.

Distillation Curve Model

The DC model is a numerically effective method, which is capable to reflect evaporation of multi-component fuel droplets without time consuming discretization of the droplet interior [8]. Within the DC model it is assumed that the temperature and chemical concentration is spatially uniform inside the droplet but both quantities will change in time. Thus an analytical model can be derived [11], which is characterized by a thermo-physical state that varies according to the ASTM distillation data for real fuels during droplet evaporation [6]. In contrast to the well-known Rapid-Mixing Model [12], diffusion resistance for a rapid droplet evaporation has been taken into account. Convective heat and mass transfer calculations of the gaseous phase are based on the well-known methods based on the Stefan flow effect [1].

Liquid Phase Droplet evaporation of real fuels like kerosene, diesel or gasoline is characterized by a distillation process. High volatile components are evaporated in the earlier stages, while low volatile species remain inside the droplet resulting in a variation of the chemical composition of the droplet. Mass diffusion is induced in the

interior of the droplet by the evaporation process causing an increasing concentration of low volatile components during the time of evaporation. The ratio of the characteristic timescales of droplet lifetime and mass diffusion has a decisive influence on the variation of the molar weight. If the droplet lifetime is short in comparison to the mass diffusion timescale, the distillation process is suppressed. In this case, the resulting molecular weight is different from the distillation curve. The influence of diffusion resistance on the evaporation is quantified by the liquid Peclet number [11],

$$Pe = \frac{\dot{m}_{vap}}{2\,\pi\,D_d\,\Gamma_l\,\rho_l}\ . \tag{1}$$

An $Pe \to 0$ describes equilibrium evaporation according to the fuel distillation curve. For $Pe \to \infty$, the diffusion within the droplet is suppressed, thus the droplet composition remains unchanged. For Peclet numbers between both limits, the molecular weight M_{vap} is calculated by an exponential interpolation equation [11],

$$\begin{aligned} M_{vap} &= M_{vap,Pe\equiv\infty} + \left(M_{vap,Pe\equiv 0} - M_{vap,Pe\equiv\infty}\right) e^{-(C\,Pe)}, \\ \text{with} \quad & C = 0.305\,\Omega - 0.35\,\Omega^2 + 0.14\,\Omega^3. \end{aligned} \tag{2}$$

Variable C is a function of the evaporated droplet mass fraction Ω determined by DL model calculations [11]. $M_{vap,Pe\equiv 0}$ is approximated by the Legendre polynomial (3) derived from ASTM distillation data of real fuels [6],

$$\begin{aligned} M_{vap,Pe\equiv 0} &= c_1P_1 + c_2P_2 + c_3P_3 + c_4P4 + c_5P_5, \\ \text{with} \quad & P_1 = 1,\ P_2 = S,\ P_3 = \frac{3S^2-1}{2},\ P_4 = \frac{5S^3-3S}{2},\ P_5 = \frac{35S^4-30S^2+3}{8}, \\ \text{where} \quad & S = 1 - 2\Omega. \end{aligned} \tag{3}$$

The coefficients c_i are available for JP-4, Jet-A1 and Diesel [6]. Studies of other real fuels like high volatile and low volatile gasoline have been published [2]. $M_{vap,Pe\equiv\infty}$ is approximated by the mean value of the remaining liquid fuel (Eq. 4). This simplification is valid for low Pe numbers, typically occurring in technical combustion chambers.

$$M_{vap,Pe\equiv\infty} = \frac{\int_\Omega^1 M_{vap,Pe\equiv 0}\,d\tilde{\Omega}}{1-\Omega} \tag{4}$$

Gas phase For the application of the DC model, the gas phase is assumed to be quasi-steady. Since the characteristic timescales in the gas phase are smaller by orders of magnitude compared to the droplet interior diffusion time scales, the quasi-steady assumption is valid for a moving droplet in a high pressure environment [3]. This assumption is giving rise to a quasi-steady description of the diffusive transport processes. By using the reference values for the fluid properties ($1/3$-rule [13]), the integration of the transport equations outside the droplet for mass and enthalpy yields analytical expressions for the diffusive transport fluxes. As result, differential equations for droplet mass (Eq. 5) and temperature (Eq. 6) can be derived from mass and energy balance. Convective transport is considered by empirical correction factors cfm and cfh (Eq. 7) [5]. Additionally, the extended film theory [1] is incorporated into the DC model, in order to account for effects such as a non-unitary Lewis number and the Stefan flow effect on moving droplets. The derivation of the complete gas phase model was published previously [8].

$$\frac{dm_d}{dt} = -cfm\,2\pi D\,\rho_{g,ref}\Gamma_{g,ref}\ln\frac{1-Y_{vap,g}}{1-Y_{vap,s}} \tag{5}$$

$$\frac{dT_d}{dt} = -\frac{1}{m_d\,c_{p,d}}\frac{dm_d}{dt}\left[\frac{cfh}{cfm}c_{p,vap,ref}(T_g - T_d)\left(\left[\frac{1-Y_{vap,g}}{1-Y_{vap,s}}\right]^{\frac{1}{Le}} - 1\right)^{-1} - h_{vap}\right] \tag{6}$$

$$cfm = 1 + 0.276Re^{\frac{1}{2}}Sc^{\frac{1}{3}}\ , \quad cfh = 1 + 0.276Re^{\frac{1}{2}}Pr^{\frac{1}{3}} \tag{7}$$

In principle, a transient description of the gas phase has to be used in particular for non moving droplets evaporating in a high pressure environment [16]. The accuracy of the present quasi-steady model has been assessed by comparing the results of the DC model to the fully transient DL model. It was found that the quasi-steady approach yields good results for a typical elevated pressure application in combustion chambers at significantly reduced computational effort.

Phase change The phase change at the droplet surface is mainly affected by the fuel vapor concentration. This quantity has a decisive impact on the evaporation of a liquid droplet and has to be determined carefully. Since real fuels are a blend of several pure substances, property data can hardly be approximated by common thermo-physical correlations. Polynomial fittings for the vapor pressure derived from measurements are available [6] [2]. Combining these with Raoult's Law the vapor concentration can be determined for low pressure conditions. Since an ideal behavior of the gas and the liquid phase is assumed in Raoult's Law, this simplification cannot be used for elevated and high pressure conditions. The more complex vapor-liquid phase equilibrium has to be applied to consider the real gas behavior during phase change. It is represented by the equality of temperature and pressure, and the fugacity of each species in the gas and the liquid phase. Using the cubic Soave-Redlich-Kwong equation to calculate the fugacity [7], the phase equilibrium can be solved iteratively by the Regula Falsi method. In order to utilize this procedure in combination with the DC model, property parameters, such as T_c, p_c and ω, are interpolated of pure n-alkanes. The computational effort for the DC model is reduced by a precomputation of the phase equilibrium and a tabulation of the results.
The phase equilibrium is compared to Raoult's Law for a binary n-octane/air-system at different pressures in Fig. 1. It is obvious that Raoult's Law deviates strongly for high pressure conditions. The solution of the phase equilibrium for a constant pressure of 2 MPa and varying n-alkanes is also depicted in Fig. 1. As shown in the charts, a critical mixing point can be reached by the variation of pressure and also by the variation of the chemical composition.

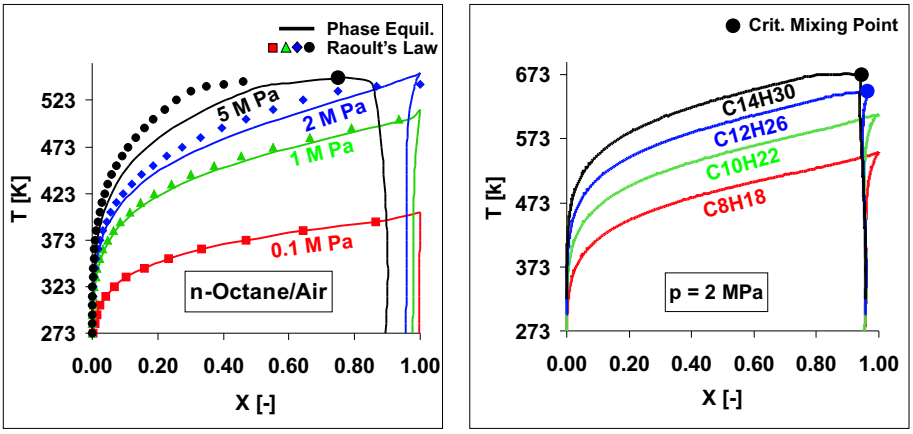

Figure 1: T-X charts for a n-octane/air-system [left] and n-alkane/air system[right]

Results and discussion

Results of the DC model are compared to experimental data as well as predicted results of the DL model. Experimental investigations of the evaporation of a single Jet-A1 droplet are still hardly available. Thus, the results of the DC model are only compared to experimental data of an evaporating JP-8 (equals Jet-A1 [9]) droplet at atmospheric conditions [10]. A validation of the DC model when predicting of the fuel preparation in an experimental LPP combustor was published previously and the predicted results were found to be in good agreement to PDA measurements [8]. Results of the DC model for a non moving Jet-A1 droplet evaporating in various stagnant environments at a temperature of 800 K and at different pressures will be presented subsequently. The results will be compared to calculations of the accurate DL model with a quasi-steady and a transient description of the gas phase. Since only two liquid fuel components can be handled by the DL model, the multi-component fuel Jet-A1 is approximated by a binary fuel mixture of 44 % n-decane and 56 % n-tetradecane. The predictions of the DL model of evaporating binary fuel droplets at high temperature and high pressure conditions was compared previously to experimental results and found in good agreement [15].

Experimental investigation The predictions of the DC model are compared to an experimental investigation in which the evaporation of a suspended JP-8 droplet in an cold air stream at atmospheric temperature and pressure was studied. In contrast to a stagnant atmosphere, forced convection is present in this case. As depicted in Fig. 2, the predicted results of the DC model agree well to the experimental data.

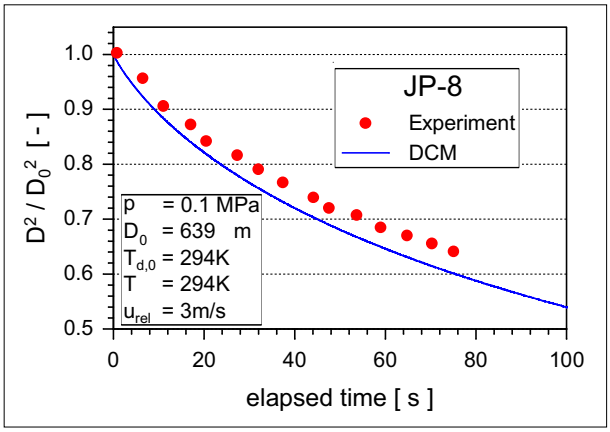

Figure 2: Comparison of predicted results of the Distillation Curve Model and experimental data for D square ratio

Liquid phase modeling In order to assess the accuracy of the liquid phase modeling, a comparison is made to the DL model with the additional assumption of a quasi-steady gas phase. Only the interior of the droplet is discretized and the one dimensional unsteady differential equations are solved [14]. This way, deviations caused by high pressure effects occurring in the gas phase are excluded.

The predictions of an evaporating Jet-A1 droplet at ambient pressures of 0.1, 1 and 5 MPa were computed by the DC model and compared to the DL model. The results for surface temperature, D-square ratio and vapor mass flow as a function of time are depicted in Fig. 3. Since the DC model accounts for varying Peclet numbers, the results agree well to the DL model. Regarding the mass flow rate for a pressure of 0.1 and 1 MPa a faster increase of the vapor mass flow is predicted by the DC model compared to the DL model. Since the DC model reflects experimental investigations at atmospheric pressures [8], this deviation is caused by the usage of different model fuels. Whereas a binary fuel mixture is used within the DL model, the DC model is based on a finite discretization of the molar weight, in order to reflect the distillation curve of Jet-A1. This influence of the model fuel is superposed by another high pressure effect (p = 5 MPa). Since the DC model is based on an uniform temperature profile in the droplet interior, it is only valid for low Biot numbers. If the Biot number is increasing, the assumption of an uniform temperature yields to a decreasing mass flow rate at the beginning and an increasing mass flow rate at the final part of the droplet evaporation process. In contrast to the DC model, the energy equation as function of the radial Co-ordinate is solved within the DL model for the droplet interior and , thus, a radial temperature profile can be established. This thermo-physical exact approach is valid for all Biot numbers. Since Biot numbers increase at high ambient temperature and pressure conditions, the mass flow rate as predicted by the DC model shows deviations. As the Biot number is linear to the droplet diameter, this effect can be neglected for small droplet diameters typically being present in combustion chambers.

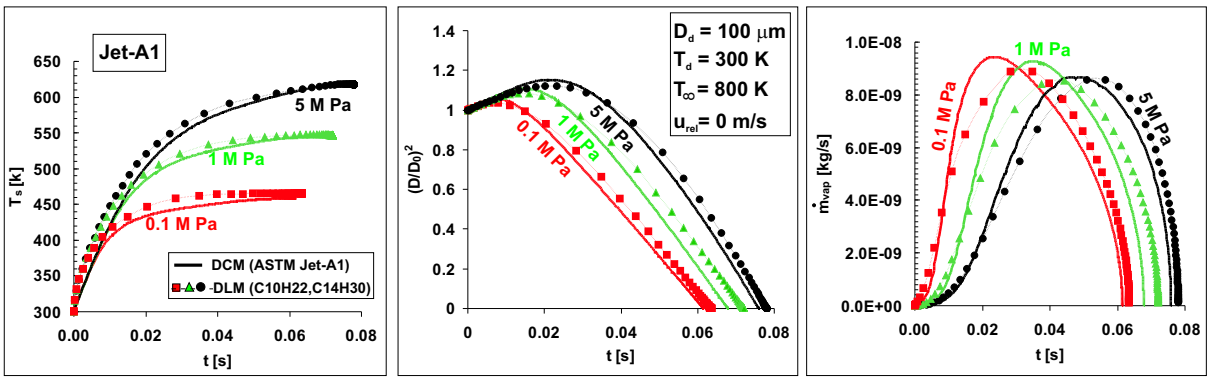

Figure 3: Comparison of predicted results of the Distillation Curve Model and Diffusion Limit Model assuming a quasi-steady gas phase for surface temperature, D square ratio and vapor mass flow

Gas phase modeling The influence of transient effects during the droplet evaporation process is studied in this section. The results of the DC model are compared to the DL model. A transient description of the gas phase is used within the DL model by solving the system of unsteady differential equations for the surrounding gas and liquid phase of the droplet. Predicted results of the DC model and the fully transient DL model for ambient pressures of 0.1, 1 and 2 MPa are plotted in Fig. 4.
Transient effects have a decisive influence at the beginning of the droplet evaporation process at atmospheric as well as at elevated pressures. Whereas an immediate increase of the vapor mass flow is predicted by the fully transient DL model, the quasi-steady DC model yields a delay of the vaporization process. This deviation of transient and quasi-steady gas phase modeling increases strongly at higher ambient pressures. Nevertheless, DC model shows quite good accuracy at low and elevated pressures (P = 2 MPa). It has to be emphasized, that the transient description of the gas phase is only necessary when natural heat and mass convection is predominant like in this test case. In case of forced convection by relative velocities of moving droplets, the quasi-steady description combined with a convective correction is sufficient [3].

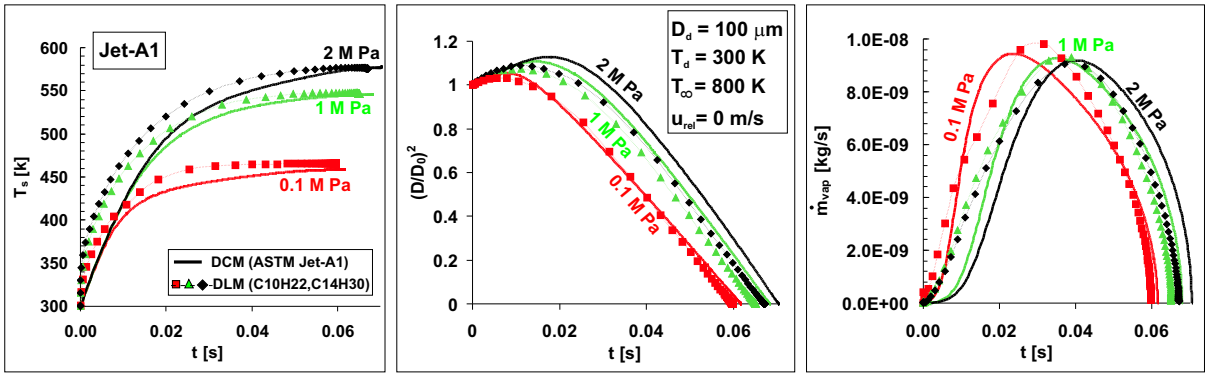

Figure 4: Comparison of predicted results of Distillation Curve Model and fully transient Diffusion Limit Model for surface temperature, D square ratio and vapor mass flow

Computational efficiency The computational efficiency of the DC model and the DL model will be compared subsequently. For a meaningful comparison, the DC model is studied with and without using pre-tabulated thermo-physical property data. The computational effort for the DL model assuming a transient and quasi-steady description of the gas phase is also studied separately. The results are presented in Table 1.

Model	CPU time [s]
DC model with lookup tables	0.280
DC model without lookup tables	11.08
DL model assuming quasi-steady gas phase	106.2
DL model assuming transient gas phase	965.4

Table 1: CPU time [900 MHz Athlon] in comparison

Since the DC model is based on an analytical description, about ten times less computational time is required compared to the DL model assuming a quasi-steady gas phase model. The computational effort can be reduced by a factor of forty by using lookup tables for thermo-physical properties. Thus, the DC model combined with lookup tables performs best. A tremendous computational effort for the prediction is required by the fully transient DL model due to the need of a fine discretization for the gas and the liquid phase.

Conclusion

In the present paper a new computational effective droplet evaporation model has been presented which is specifically suitable for multi-component fuels and can be applied at atmospheric as well as at elevated pressures . The model is based on the distillation curve of multi-component fuels like kerosene, diesel or gasoline. It is capable to account for slow as well as rapid evaporation by an empirical correlation. In order to improve the computational

efficiency of the model, thermo-physical properties have been precomputed and lookup tables have been generated. The predicted results have been compared to the semi and fully transient DL model. The results of the present DC model are in good agreement to the DL model at different pressure conditions.
The DC model provides accurate results for multi-component droplet evaporation in technical combustors. Due to its high computational efficiency, this model is suitable for the implementation in a CFD code. This way, the two phase flow in combustion chambers at elevated pressure conditions can be predicted with reasonable computational effort.

Acknowledgments

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