



Droplet evaporation modeling by the distillation curve model: accounting for kerosene fuel and elevated pressures

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Abstract

The emission of jet engines is strongly affected by the fuel preparation process. Due to stringent emission standards, the development of low emission combustor concepts, like lean premixed prevaporized combustion or rich quench lean burn, is an important goal. For the design process of advanced combustors, numerical methods become more and more important. In order to provide an accurate prediction of the fuel preparation process, an exact numerical prediction of thermophysical processes is crucial.

A numerically effective fuel droplet evaporation model is presented in the present paper which accounts for the description of multi-component fuels like kerosene. Fractional boiling is described by a single process variable: the molar weight. This way, the fractional distillation process during evaporation of kerosene droplets is taken into account. In addition, a novel method for modeling the properties of the fuel is provided: the property data are supplied as a function of the molar weight. Real gas effects are also taken into account, in order to achieve an accurate prediction at elevated pressures.

The major advantage of this new model is that algebraic expressions are derived for the multi-component droplet vaporization. Thus, the present model combines both numerical efficiency and accuracy.

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Keywords: Fuel droplet; Multi-component fuel; High pressure evaporation

1. Introduction

Fuel droplet evaporation models have been investigated by a number of authors for several decades. Due to its simplicity the D^2 -model [23] was often used in past times. However, its applicability to technical sprays is strongly limited [3,14]. The Rapid Mixing Model [6] is presently the more common model. Within this model, the assumption is made that the different components of a multi-component fuel are completely mixed inside the

droplet during its lifetime. Additionally, a uniform temperature distribution is assumed for the liquid phase throughout the evaporation process. Therefore, this model is limited to an infinite fast transport of heat and mass [21,22]. Predictions may be inaccurate, because the assumption of rapid diffusion is not valid for kerosene droplets in particular at elevated pressures [26].

Reasonable results for practical spray predictions can be achieved by the Diffusion Limit Model (DL model) [12,21]. Within this model approach, heat and mass transfer in radial direction inside the droplet is accounted for. The DL model is valid for low and high pressure applications [10,25] but the number of fuel components is limited. Thus, the prediction of real aviation fuels consisting of several hundreds of pure components is still problematic. An improved model

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Nomenclature

a	SRK parameter, $\text{N m}^4/\text{mol}^2$
b	SRK parameter, m^3/mol
$B_{M,T}$	Spalding numbers
D	diameter, m
h	specific enthalpy, J/kg
J_A	Jamieson parameter A
J_B	Jamieson parameter B
k	binary constant
Le	Lewis number
m	mass, kg
M	molar weight, kg/mol
Nu	Nusselt number
p	pressure, Pa
P_n	Legendre polynomial
Pe	Peclet number
R	universal gas constant, J/mol K
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
t	time, s
T	temperature, K
u	velocity, m/s
v	molar volume, m^3/mol
x	variable
X	molar fraction
Y	mass fraction, kg/mol
Z	real factor

Greek symbols

α	SRK parameter
Γ	diffusion coefficient, m^2/s
φ	fugacity coefficient
Φ	property parameter, gen.
ω	acentric factor
Ω	evaporation mass fraction

Subscripts

0	initial
*	characteristic
b, c	boiling, critical
d, g	droplet, gas
l, vap	liquid, vapor
m	mean, mixture
r	reduced
ref	reference
rel	relative
s	droplet surface

Abbreviations

AVE	average
DC	distillation curve
DL	diffusion limit
LPP	lean premixed prevaporized
PDA	phase doppler anemometry
RQL	rich quench lean
SRK	Soave–Redlich–Kwong

approach accounting for complex fuel mixtures by using continuous thermodynamics is available [26,27]. Despite being quite accurate both models are based on differential equations describing the exchange in radial direction within the droplet. Thus, these models are expensive in computation, and therefore, they are less suitable for multiphase flow predictions in combustors. That is the reason, why simple models, like the rapid mixing model, are still being used in applied CFD codes. The major objective of this paper is to present a numerical effective evaporation model which is applicable to the quantitative prediction of kerosene sprays in combustion chambers.

This new, computational effective multi-component evaporation model, the Distillation Curve Model (DC model) is capable to reflect the distillation curve of aviation fuels, like JP-4, Jet-A1 and diesel. The major feature of the DC model is to describe fractional boiling during the droplet vaporization 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 algebraic equations. Thus, the computational effort of the DC model is lower by orders

of magnitudes compared to complex models based on differential equations.

Inherent to presently available droplet evaporation models is the restriction of relying on a model fuel consisting of a few components. Since kerosene is a blend of several hundred species, a model fuel is required which accounts for the thermophysical properties of a complex multi-component fuel mixture. A novel model fuel has been incorporated into the DC model by which the variation of the molar weight during droplet evaporation is mimicked according the real fuel under consideration. The actual properties of the model fuel have been derived from the properties of n -alkanes. In order to take into account high pressure effects, real gas effects are also considered within the correlations and mixing rules. Additionally, the liquid–vapor phase equilibrium has been incorporated to the DC model. This way, the previously published DC model for multi-component aviation fuels [16] is adapted to elevated pressures and temperatures which are typical for technical combustion chambers.

In the paper, a comparison of the results predicted by the DC model to those of the rather accurate DL model is presented for atmospheric and elevated pressures. The

operative range of the DC model is discussed for varying pressure conditions.

The results reveal that, in contrast to complex and numerical expensive single droplet vaporization models, the DC model achieves both high accuracy and numerical efficiency. By implementing the DC model into multi-phase CFD codes, the fuel preparation process of kerosene sprays can be predicted efficiently and accurately in technical combustion chambers.

2. Distillation curve model

The DC model is a numerically effective method, which is capable to reflect the evaporation of multi-component fuel droplets without discretization of the droplet interior and without a time consuming solution of transport equations [16]. 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 algebraic model can be derived [20] which is characterized by a thermo-physical state that varies according to the ASTM (American Society for Testing and Materials) distillation data for real fuels during droplet evaporation [8]. In contrast to the well-known rapid-mixing model [21], 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 assuming the Stefan flow [2].

2.1. 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 time scales 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 time scale, 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 [15]

$$Pe = \frac{\dot{m}_{\text{vap}}}{2\pi D_d \Gamma_1 \rho_1} \quad (1)$$

$Pe \rightarrow 0$ describes equilibrium evaporation according to the fuel distillation curve. For $Pe \rightarrow \infty$, 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 [20],

$$M_{\text{vap}} = M_{\text{vap},Pe=\infty} + (M_{\text{vap},Pe=0} - M_{\text{vap},Pe=\infty})e^{-(C Pe)},$$

with $C = 0.305\Omega - 0.35\Omega^2 + 0.14\Omega^3$,

and $\Omega(t) = 1 - \frac{m_d(t)}{m_{d,0}}$. (2)

The variable C is a function of the evaporated droplet mass fraction Ω . It is determined from DL model calculations [12,15,20]. $M_{\text{vap},Pe=0}$ is approximated by a Legendre polynomial [Eq. (3)] derived from ASTM distillation data of real fuels [8]

$$M_{\text{vap},Pe=0} = c_1 P_1 + c_2 P_2 + c_3 P_3 + c_4 P_4 + c_5 P_5,$$

with $P_1 = 1$, $P_2 = S$, $P_3 = \frac{3S^2 - 1}{2}$, $P_4 = \frac{5S^3 - 3S}{2}$,

$P_5 = \frac{35S^4 - 30S^2 + 3}{8}$, where $S = 1 - 2\Omega$. (3)

The coefficients c_i are summarized for Jet-A1 in Table 1. Polynomial fittings are also available for JP-4 and Diesel [8]. Studies of other real fuels like high volatile and low volatile gasoline have been published [4].

$M_{\text{vap},Pe=\infty}$ is depending on the droplet history and has to be approximated by the mean value of the non-vaporized liquid fuel during the calculation [Eq. (4)]. The derivation of this approach was already published and described in detail [20].

$$M_{\text{vap},Pe=\infty} = M_{\text{vap,AVE}} = \frac{\int_{\Omega}^1 M_{\text{vap},Pe=0} d\tilde{\Omega}}{1 - \Omega} \quad (4)$$

Predicted results of molecular weight and Peclet number for an evaporating Jet-A1 droplet at different ambient pressures are depicted in Fig. 1. The results reveal that the variation of the ambient pressure has a decisive influence on the characteristic time scales of the evaporation process.

2.2. Phase change

The fuel vapor concentration at the droplet surface is influenced by the phase change. This vapor concentration

Table 1
Coefficients for use with Legendre polynomial [Eq. (3)] [8]

Fuel	c_1	c_2	c_3	c_4	c_5
Jet-A1	1.7337E2	-1.4785E1	-1.0524	-8.5762E-1	-1.0516

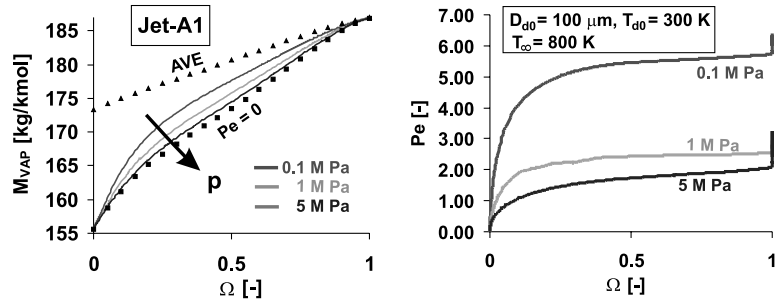


Fig. 1. Molecular weight of the fuel vapor (left) and the liquid phase Peclet number (right) for an Jet-A1 droplet, predicted by the DC model.

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 thermophysical correlations. Polynomial fittings for the vapor pressure derived from measurements are available [4,8]. 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 high pressure conditions. The more complex vapor–liquid phase equilibrium has to be applied to consider the real gas behavior during phase change [25,26]. In order to utilize this procedure in combination with the DC model, a model fuel has to be created containing all required property parameters.

2.3. Gas phase

For the application, the quasi-steady gas phase model [6] is incorporated into the DC model. In case of forced convection, the characteristic time scales in the gas phase are smaller by orders of magnitude compared to the droplet interior diffusion time scales. Thus, transport processes in the gas phase can be assumed to be quasi-steady for each time interval during integration. The quasi-steady assumption is valid for a moving droplet even in a high pressure environment [5] and 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 [24]), 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 a mass and energy balance [2,6]

$$\frac{dm_d}{dt} = -\pi D_d \rho_{g,ref} \Gamma_{g,ref} Sh^* \ln(1 + B_M) \quad (5)$$

$$\frac{dT_d}{dt} = -\frac{\dot{m}_{vap}}{m_d c_{p,d}} \left(\frac{c_{p,vap,ref}(T_g - T_d)}{B_T} - h_{vap} \right) \quad (6)$$

The Spalding heat and mass transfer numbers B_M and B_T are calculated as

$$B_M = \frac{Y_{vap,s} - Y_{vap,g}}{1 - Y_{vap,s}} \quad (7)$$

and

$$B_T = (1 + B_M)^x - 1, \quad x = \frac{c_{p,vap,ref}}{c_{p,g,ref}} \frac{Sh^*}{Nu^*} \frac{1}{Le} \quad (8)$$

Convective transport is considered by a modified Sherwood and Nusselt number. A good approximation of the parameters Sh^* and Nu^* is given by the well-known Frössling correlations [Eq. (9)] [7].

$$Sh^* = 2 + 0.552 Re^{1/2} Sc^{1/3}, \quad Nu^* = 2 + 0.552 Re^{1/2} Pr^{1/3} \quad (9)$$

This approximation can be improved by the extended film theory [2] which accounts for additional effects, such as a non-unitary Lewis number and the Stefan flow in case of a moving droplet [3,22]. The derivation of the complete gas phase model incorporated into the DC model was published previously [16].

In case of free heat and mass convection, the assumption of a quasi-steady gas phase is not entirely valid. Gas phase unsteadiness exits during the early period of the vaporization process in particular in high pressure environments [27]. An exact prediction can only be achieved by a transient description of the gas phase. 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 predicting a non-moving Jet-A1 droplet. Despite neglecting gas phase unsteadiness, the quasi-steady approach yields good results at significantly reduced computational effort.

3. Model fuel

Real aviation fuels are a mixture of several hundreds of pure components of different molar weight. As shown in Fig. 2, the molar weight of the pure hydrocarbons

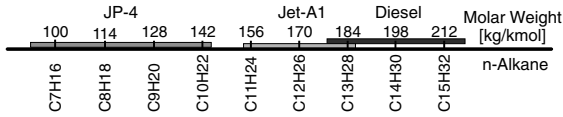


Fig. 2. Molar weight of pure *n*-alkanes and real aviation fuels.

contained in real aviation fuels varies over a wide range [17].

If the evaporation of multi-component fuel droplets are predicted by the DC model, the volatility of the fuel is taken into account by the variation of the molar weight by the corresponding mixture of *n*-alkanes. This simplification is valid, if the evaporation of the real fuel is governed by the *n*-alkanes. A new model fuel is proposed in this study which provides thermophysical properties as function of the molar weight. The basic concept within this model fuel is that properties of all *n*-alkanes contained in the real fuel can be determined by the same correlations summarized in Table 2. Only the property parameters, like T_c , p_c , etc. are characteristic for the specific *n*-alkane. In order to correlate the

property data as a function of the molar weight, an interpolation procedure is used. The principle of the interpolation of the property parameters as well as the polynomial of T_c is illustrated in Fig. 3.

The dependency on the molar weight of various property parameters is approximated by a polynomial function [Eq. (10)] according to the data of pure *n*-alkanes [1,18]. The polynomial fittings are valid for a range of $M = 30$ kg/k mol (C_2H_6) up to $M = 282$ kg/k mol ($C_{20}H_{42}$).

$$\Phi(M) = f(x), \quad x = A + B \cdot M + C \cdot M^2 + D \cdot M^3 + \frac{E}{M} \quad (10)$$

The coefficients of Eq. (10) are summarized in Table 3.

4. Vapor–liquid phase equilibrium

The vapor–liquid phase equilibrium is described by the expression

Table 2
Thermophysical properties

Property	Correlation	Pressure correction
<i>Liquid phase</i>		
Density	Hankinson and Thomson [18]	Thomson [18]
Heat capacity	Polynomial 3. order [18]	Rowlinson [18]
Dynamic viscosity	Van Velzen, Letsou and Stiel [18]	Lucas [18]
Thermal conductivity	Jamieson [18]	Lenoir [18]
Enthalpy of evaporation	Soave-Redlich-Kwong [9]	Soave-Redlich-Kwong [9]
Diffusion coefficient	Wilke-Chang [18]	–
<i>Gas phase</i>		
Density	Soave-Redlich-Kwong [9]	Soave-Redlich-Kwong [9]
Heat capacity	Polynomial 3. order [18]	Lee and Kesler [18]
Dynamic viscosity	Lucas [18]	Lucas [18]
Thermal conductivity	Roy and Thodos, Wassiljeva [18]	Stiel and Thodos [18]
Diffusion coefficient	Fuller [18]	Takahashi [18]

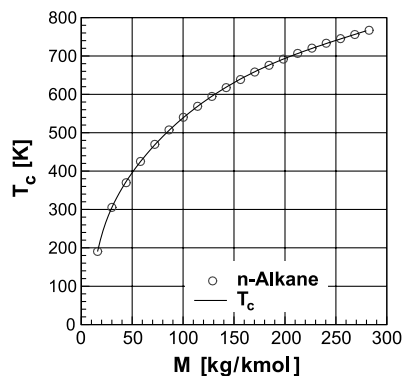
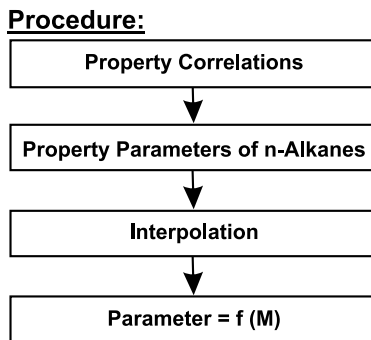


Fig. 3. Interpolation procedure for the model fuel (left) and the polynomial fitting for the critical temperature (right).

Table 3
Coefficients of the polynomial interpolation function of the property parameters

Φ	$f(x)$	A	B	C	D	E
ω	$\frac{x}{T_c}$	-7.046E1	2.539E3	5.941E2	1.104E2	5.132E-1
T_c	x	2.768E2	3.844E3	-1.132E4	1.404E4	2.330
p_c	$1.E6 \cdot e^x$	1.776	-1.0182E1	2.511E1	3.738E1	3.507E-3
Z_c	x	2.904E-1	-3.419E-1	6.042E-1	0	0
v^*	x	3.860E-5	3.475E-3	4.333E-3	0	0
J_A	x	4.505E-2	-2.496E-2	3.408E-1	0	0
J_B	x	5.321	-2.919E1	5.968E1	0	0

$$X_i^l \phi_i^l = X_i^g \phi_i^g. \quad (11)$$

If each component has the same temperature, pressure and fugacity in the gas and in the liquid phase, the phases are in equilibrium state. The cubic SRK equations are suitable for calculating the fugacity in both phases [9]. The fugacity coefficients ϕ_j are given by the function

$$\ln \phi_j = \ln \frac{v}{v - b_m} - \frac{2 \sum_i X_i a_{ij}}{RTb_m} \ln \frac{v + b_m}{v} + \frac{b_j}{v - b_m} - \ln \frac{pv}{RT} + \frac{ab_j}{RTb_m^2} \left(\ln \frac{v + b_m}{v} - \frac{b_m}{v + b_m} \right) \quad (12)$$

$$a = 0.42748 \cdot \frac{R^2 T_c^2}{p_c} \cdot \alpha, \quad b = 0.08664 \cdot \frac{RT_c}{p_c}. \quad (13)$$

In order to determine the coefficients α , a_m , b_m of the fuel/air mixture, mixing rules for the SRK equations are provided by the following expressions:

$$\alpha = \left[1 + (0.48 + 1.574\omega - 0.176\omega^2) \left(1 - \left(\frac{T}{T_c} \right)^{0.5} \right) \right]^2 \quad (14)$$

$$a_m = \sum_{i=1}^n \sum_{j=1}^n X_i X_j \sqrt{a_i a_j} (1 - k_{ij,SRK}), \quad b_m = \sum_{i=1}^n X_i b_i. \quad (15)$$

Including the polynomial fittings of the model fuel for T_c , p_c and ω , the phase equilibrium can be solved for a wide range of n -alkanes by varying the molar weight. This way, high pressure effects at the droplet surface are taken into account. The phase equilibrium has no analytical solution. The system of equations is solved iteratively by the Regula Falsi method. In order to reduce the computational effort for the DC model, the solution of the phase equilibrium is precomputed and tabulated as function of temperature, pressure and molar weight (model fuel).

At a atmospheric pressure the assumption of an ideal behavior of the gas phase and the liquid phase is valid and the phase equilibrium can be approximated by Raoult's law,

$$X_i^l p_{vap,i} = X_i^g p_{system}. \quad (16)$$

In Fig. 4 the phase equilibrium is compared to Raoult's law for a binary n -octane/air system at different pressures. It is obvious that Raoult's law deviates strongly at pressures higher than 1 MPa. The solution of the phase equilibrium for a constant pressure of 2 MPa and varying n -alkanes is also depicted in Fig. 4. As shown in the charts, a critical mixing point can be obtained by the variation of pressure and also by the variation of the n -alkane, respectively, the molar weight of the model fuel.

5. Thermophysical properties

The thermophysical properties of the gas and the liquid are required for the calculation of an evaporating fuel droplet. Suitable correlations of high pressure conditions have to be used. Since fuel/air mixing takes place in the gas phase, mixing rules are required for determination of the property data of the gas phase. All property correlations used within the DC model are summarized in Table 2.

Using polynomial fittings for the property parameters of the model fuel, property data are correlated over a wide range of n -alkanes. Since high pressure property correlations and mixing rules are expensive in computation, the property data have been arranged in a lookup table as a function of temperature, pressure, molar weight (model fuel) and molar fraction (gas phase).

6. Results and discussion

Subsequently, the results of the DC model are compared to experimental data as well as to predictions 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 droplet at atmospheric conditions [19]. A validation of the DC model when predicting the fuel preparation in an

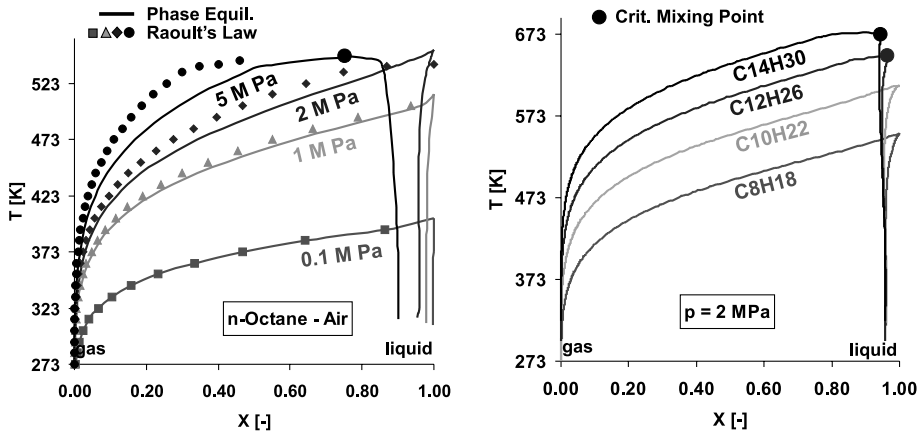


Fig. 4. T - X charts for a n -octane/air system (left) and n -alkane/air system (right).

experimental LPP combustor was published previously and the predicted results were found to be in good agreement to PDA measurements [16]. Results of the DC model for a non-moving Jet-A1 droplet under microgravity conditions evaporating in various stagnant environments at a temperature of 800 K and at different pressures will be presented subsequently. This idealized configuration is characterized by a transient spherically symmetric vaporization and can be predicted accurately by the DL model [13,21,22]. Thus, the DC model can be assessed by comparing the results to predictions of the DL model. Since the determination of mass diffusion in polynary liquid mixtures is most problematic [18], the multi-component fuel Jet-A1 is approximated by a binary mixture of 44% n -decane and 56% n -tetradecane within the DL model. 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 [12,25].

6.1. Comparison to experimental investigations

The predictions of the DC model are compared to an experimental investigation [19] in which the evaporation of a suspended JP-8 (equals Jet-A1 [17]) droplet in a cold air stream at atmospheric temperature and pressure was studied. The droplet was being subject to forced convection in this case ($u_{rel} = 3$ m/s). The experiment is well suited to validate the representation of a multi-component fuel by the DC and DL model. Predictions of both models compared to experimental data are depicted in Fig. 5. Since the DC model reflects the distillation curve of Jet-A1, the predictions agree well to the experiment. In contrast, the DL model based on a binary model fuel (44% n -decane and 56% n -tetradecane) underestimates the vaporization process during the early period.

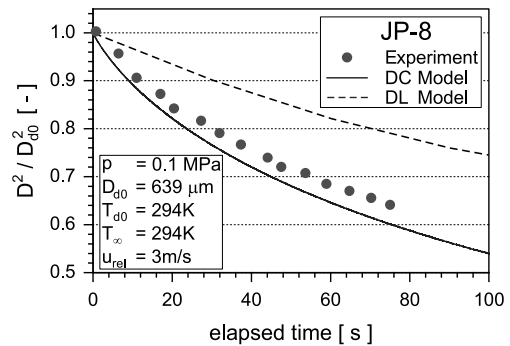


Fig. 5. Predictions of the DC model and the DL model compared to experimental data [19] (D^2 -ratio).

6.2. Assessment of 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 within the DL model [25]. This way, deviations caused by unsteady effects being present in the gas phase are excluded and the liquid phase modeling of the DC model can be assessed correctly.

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 study revealed, that only sub-critical vaporization occurs for the present cases. Although the environment is super-critical (Fig. 4), the surface temperature of the droplet is below the critical temperature of the remaining fuel components. The results for surface temperature, D^2 -ratio and vapor mass flow as a function of time are depicted in Fig. 6. Since the DC model accounts for

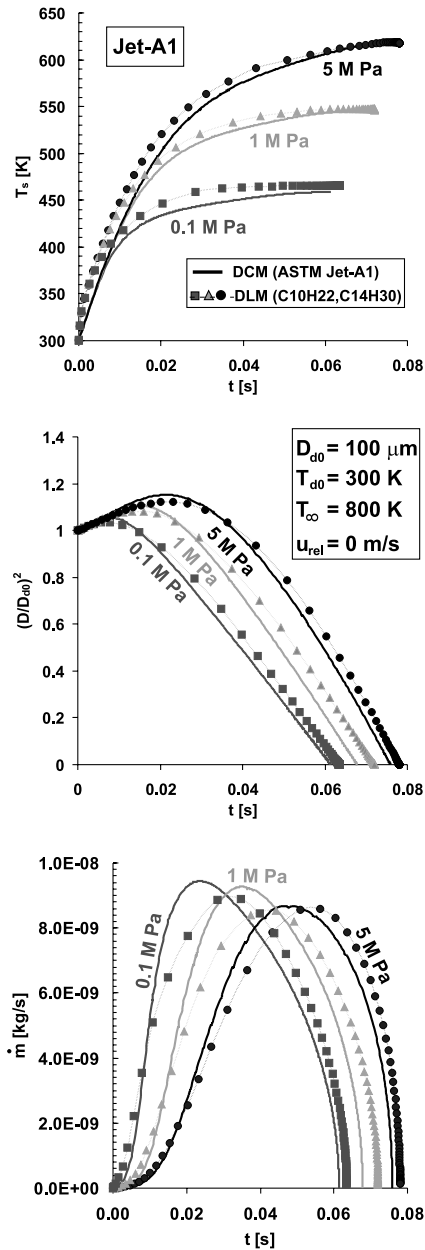


Fig. 6. Comparison of the DC model and DL model assuming a quasi-steady gas phase (surface temperature, D^2 -ratio and vapor mass flow).

varying Peclet numbers, the results for surface temperature and D^2 -ratio 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 with good accuracy (Fig. 5), the deviation of the DL model is caused by the usage of

a simpler model fuel. 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. It is obvious, that a complex fuel, like Jet-A1, cannot be approximated by a binary fuel mixture. Thus, the DL model under-predicts the mass flow rate of an evaporating Jet-A1 droplet.

The deviation caused by different model fuels is superposed by another high pressure effect. Increasing the pressure up to 5 MPa, the mass flow rate predicted by the DC model decreases stronger in comparison to predictions by the DL model. 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 mass and energy equations as function of the radial co-ordinate are solved within the DL model for the droplet interior. Thus, a radial mass fraction and temperature profile can be established. This thermophysical rather accurate approach is valid for all Peclet and 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 of gas turbines.

6.3. Assessment of 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. The theory of this model was already published [11,12]. 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. 7.

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 free heat and mass convection is predominant like in this test case. In case of

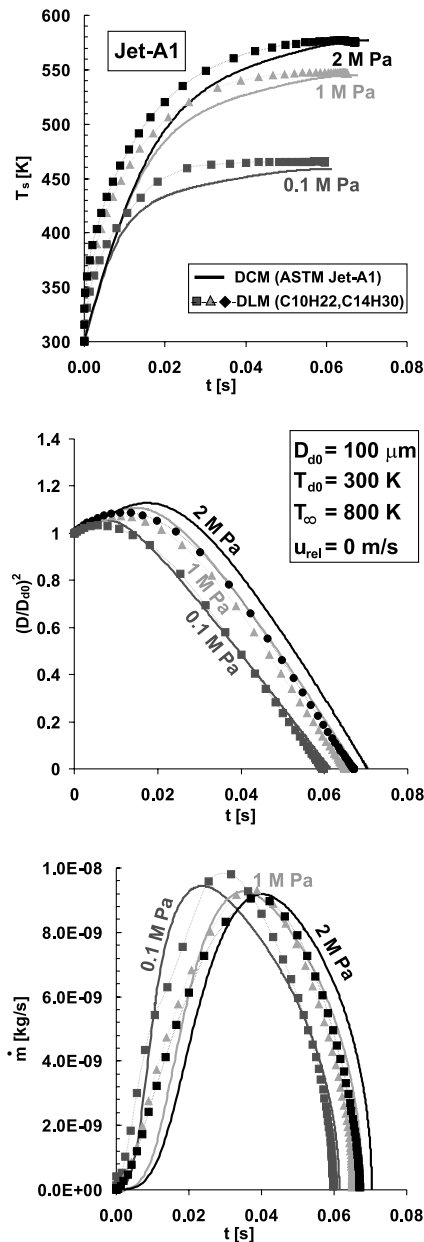


Fig. 7. Comparison of the DC model and the fully transient DL model (surface temperature, D^2 -ratio and vapor mass flow).

forced convection by relative velocities of moving droplets, the quasi-steady description combined with a convective correction is sufficient [5].

6.4. 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 also studied

Table 4
CPU time [900 MHz Athlon] in comparison

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

without using pre-tabulated thermophysical 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 4.

Since the DC model is based on algebraic equations, about 10 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 40 by using lookup tables for thermophysical properties. Thus, the DC model combined with lookup tables performs best. Because of its computational efficiency, the DC model is a suitable tool for improving the accuracy of spray predictions.

7. 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, thermophysical 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. 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.

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