A Two-Parameter Corresponding States Method for Calculating the Steady-State Evaporation Rate of C_2 – C_9 n-Alkane Droplets in Air for Elevated Pressures and Temperatures

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Abstract

Advanced gas turbine and internal combustion engine combustion chambers operate at highly elevated pressures and temperatures. Therefore, spray vaporization analysis cannot be limited to the atmospheric environment since evaporation strongly depends on ambient conditions. Presently, the effect of air pressure and temperature on droplet evaporation rate was investigated by using both a transient and a steady-state approach. A corresponding states model was derived for the steady-state evaporation rate for n-alkanes in the range of C_2 – C_9 with an excellent fit quality and < 1% model uncertainty, considering the thermo-physical data uncertainties. The model was tested for C_1 , C_{10} , and C_{12} n-alkanes as well with low success. The ambient conditions were evaluated in terms of reduced pressures and temperatures, covering the range of 0.02–0.5 and 1.2–1.5, respectively. However, the applicability of the model was limited to reduced temperature of 1.3–1.5, as higher discrepancy was observed between the trends of the different n-alkanes at lower temperatures. Since the heat-up phase of practical sprays in combustion chambers is often short, the present model might significantly reduce the computational effort required for liquid evaporation calculations.

Keywords Droplet · Vaporization · Evaporation · n-alkane · Pressure · Temperature

List of Symbols

Latin Letters

B_M	Spalding mass transfer number
B_T	Spalding heat transfer number
c_p	Specific heat capacity at constant pressure

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D	Binary diffusion coefficient
d	Droplet diameter
Gr	Grashof number
k	Thermal conductivity
L	Latent heat of vaporization
Le	Lewis number
$\dot{m}_d$	Mass flow rate of vapor at the droplet surface
M	Molar mass
Nu	Nusselt number
p	Pressure
Ra_M	Rayleigh number for mass transfer
Ra_T	Rayleigh number for heat transfer
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
T	Temperature
t	Time
Y	Mass fraction

Greek Symbols

β	Thermal expansion coefficient of mixture
Λ	Non-dimensional evaporation rate
λ	Evaporation rate
μ	Dynamic viscosity
ρ	Density
σ	Deviation

Subscripts

0	Initial value
15%	15% of the initial value
∞	Ambient
a	Air
bn	Normal boiling point
c	Critical
d	Droplet
g	Fuel vapor-air mixture
l	Liquid
r	Reduced value
s	Surface of droplet
st	Steady-state
v	Fuel vapor

1 Introduction

The dependence of the energy and transportation sectors on combustion systems is significant. The fossil fuel utilization has been rapidly increasing. Especially in the Asian and African countries, reaching a share of 85–90% in the last decades (Kibria et al. 2019).

Also, aviation has no alternative in the short term (Chiaramonti 2019). As renewable liquid fuel utilization is increasing, catalytic synthesis of n-alkanes from clean synthesis gas is gaining more importance (Deneyer et al. 2015; Lødeng et al. 2018).

Methane is the most promising liquid-propellant in the space industry (Pérez-Roca et al. 2019). N-butane is popular in spark-ignition engines to improve mixture formation (Jung et al. 2017). Evaporation and combustion of n-hexane, n-heptane, and n-octane are often investigated since their thermophysical and chemical properties are well-known (Pal and Bakshi 2018; Wu et al. 2019; AlZahrani and Dincer 2017). N-dodecane is the best one-component surrogate of diesel oil (Savard et al. 2019; Borghesi et al. 2018). Furthermore, n-alkanes are present in all gasoline, kerosene, and diesel fuels (Deneyer et al. 2015). Ray and Raghavan (Ray and Raghavan 2020) determined a correlation for the time-averaged evaporation rate of several biodiesels. Similarly, the present paper aims to provide a method for calculating the steady-state evaporation rate, based on the law of corresponding states (LCS) for a range of n-alkanes to speed up the numerical droplet evaporation simulations.

The missing material properties in heat and mass transfer calculations are often patched by group contribution methods (GCM) and LCS (Poling et al. 2001). Normal boiling point and critical parameter estimation methods were proposed by Joback (Joback (1984); Joback and Reid 1987) and Constantinou et al. (Constantinou and Gani 1994; Constantinou et al. 1995). Chung et al. (1984,1988) and Svehla (1962) provided methods for vapor-phase thermal conductivity, while Elbro (Elbro et al. 1991) suggested a method for liquid-phase density. Nevertheless, droplet lifetime calculations may show an outstanding sensitivity on them, even though the estimation method provides sufficient prediction (Csemány and Józsa 2017). Consequently, vaporization calculation requires a continuum-based analysis.

A milestone in droplet evaporation research was the introduction of the d^2 -law (Spalding 1953; Godsave 1953). In steady-state evaporation, the square of droplet diameter decreases linearly with time. Its slope is the steady-state evaporation rate that characterizes the intensity of the vaporization process (Lefebvre and McDonell 2017). State-of-the-art numerical methods are based on the aforementioned classical models (Fang et al. 2019; Ciottoli et al. 2020; Poulton et al. 2020). However, several unsolved problems have been still existing; therefore, improving, testing, and validating vaporization models are critical even today (Sazhin 2017; Pinheiro and Vedovoto 2019).

To better understand the physical phenomena of evaporation and validate vaporization models, single droplet measurement is usually performed. A rich experimental study was performed by Ghassemi et al. (Ghassemi et al. 2006) for millimeter-scale single droplets at varying ambient conditions. Nomura et al. (2017) investigated the pressure dependence of the droplet lifetime and the evaporation rate of n-hexadecane droplets in sub- and supercritical conditions in microgravity. Chauveau et al. (2011) analyzed the validity of the d^2 -law in case of n-decane droplet vaporization in microgravity and normal gravity conditions and then compared the droplet lifetime. Verwey and Birouk (2018) investigated the effect of natural convection on the steady-state evaporation rate of n-alkane droplets, while Nguyen et al. (2018) studied binary mixture droplets in a hot convective environment numerically with experimental validation. Hillenbrand and Brüggemann (Hillenbrand and Brüggemann 2020) applied non-intrusive optical measurement techniques to determine the vaporization characteristics of several alkane-ethanol mixtures and evaluated their mixture formation behavior.

The present paper aims to compare the evaporation characteristics of various n-alkanes in the range of C_1 – C_{12} for a wide range of ambient pressures and temperatures to draw general conclusions. Since the share of the heat-up period of the typical droplet sizes (5–20 μm (Lefebvre and McDonell 2017; Urbán et al. 2019)) in real combustion chambers

is relatively small, steady-state evaporation phase of n-alkanes was emphasized. Beyond the direct application of the model for fossil fuels, if a mixture of these n-alkanes can substitute the distillation curve of any other liquid, then the method is still applicable for the estimation of vaporization.

2 Materials and Methods

The presently used droplet evaporation model is detailed in the literature (Lefebvre and McDonell 2017; Fuchs 1959; Sazhin 2014) and used in numerical codes (Ansys Fluent Theory Guide 2020). Therefore, this section overviews only the key equations of both transient and steady-state models. The equations below were solved in each time-step in the former case; thus the temporal variation of droplet diameter, thermophysical properties, droplet surface temperature, and evaporation properties could be obtained. Note that the droplet temperature in this analysis was uniform. The validation of the calculation method is presented in "Appendix 1" for the current parameter regime.

2.1 The Evaporation Models

Firstly, the core of the transient model is described. The mass fraction of fuel vapor on the droplet surface, assuming vapor–liquid equilibrium and ideal gas conditions, is given by Eq. (1):

$$Y_{v,s} = \left[1 + \left(\frac{p_\infty}{p_{v,s}} - 1 \right) \frac{M_a}{M_v} \right]^{-1} \quad (1)$$

where p_∞ and $p_{v,s}$ are the ambient and vapor pressures, and M is the molar mass. Subscripts a and v refer to air and vapor, respectively. Equation (1) is valid only when the compressibility factor of the gas mixture is close to unity. Otherwise, a proper equation of state must be used to calculate phase equilibria on the droplet surface (Lopez-Echeverry et al. 2017). In the present calculations, Eq. (1) is used, and the justification of its application is presented in Sect. 3. The Spalding mass and heat transfer numbers are calculated by Eqs. (2) and (3) (Sazhin 2014; Abramzon and Sirignano 1989):

$$B_M = \frac{Y_{v,s} - Y_{v,\infty}}{1 - Y_{v,s}} \quad (2)$$

$$B_T = (1 + B_M) \frac{c_{p,v}}{c_{p,g}} \frac{1}{Le} - 1 \quad (3)$$

where $Y_{v,\infty}$ is the vapor mass fraction in the far-field. Presently, $Y_{v,\infty} = 0$. $c_{p,v}$ and $c_{p,g}$ are the vapor and vapor-air mixture specific heat capacities, respectively. Le is the Lewis number, which is defined by Eq. (4):

$$Le = \frac{k_g}{\rho_g D_{v,a} c_{p,g}} \quad (4)$$

where k_g and ρ_g are the thermal conductivity and density of vapor-air mixture respectively, and $D_{v,a}$ is the binary diffusion coefficient of vapor and air, estimated by the method of Fuller (Fuller et al. 1966,1969):

$$D_{v,a} = \frac{0.00143 T_{ref}^{7/4}}{p_{\infty} M_{v,a}^{1/2} \left[(\Sigma_v)^{1/3} + (\Sigma_v)_a^{1/3} \right]^2} \cdot 10^{-4} \quad (5)$$

where T_{ref} is the reference temperature, $M_{v,a}$ is the average molar mass of the mixture substances, Σ_v is the sum of atomic and structural diffusion volume increments of the corresponding molecules. For calculating heat transfer, the Nusselt number of the droplet is:

$$Nu = \frac{\ln(1 + B_T)}{B_T} Nu_0 \quad (6)$$

where Nu_0 is the Nusselt number for a non-evaporating sphere. There are several correlations exist for Nu_0 calculation of both stagnant and moving droplets, accounting for natural and forced convection, respectively (Sazhin 2014; Springer 2010). Such correlations are shown by Eqs. (7) and (10):

$$Nu_0 = 2 + 0.56 \left(\frac{Pr Ra_T}{0.846 + Pr} \right)^{1/4} \quad (7)$$

$$Ra_T = Gr \cdot Pr \quad (8)$$

$$Gr = \frac{g \rho_g \beta (T_s - T_{\infty}) d^3}{\mu_g} \quad (9)$$

$$Nu_0 = 2 + 0.6 Re^{1/2} Pr^{1/3} \quad (10)$$

where Pr is the Prandtl number, Ra_T is the Rayleigh number of a stagnant sphere for heat transfer, Gr is the Grashof number, g is the gravitational acceleration, β and μ_g are the thermal expansion coefficient and dynamic viscosity of the vapor-air mixture, respectively, T_s and T_{∞} are the droplet surface and ambient temperatures, respectively, d is the instantaneous droplet diameter, and Re is the Reynolds number of the moving spherical droplet. Equation (10) is the Ranz-Marshall Correlation, used extensively in spray simulations. Nusselt number is the ratio of convective to conductive heat transfer at the droplet surface.

Sherwood number is the ratio of convective mass transfer rate to diffusion rate. As a result of the analogous form of the fundamental equations in heat and mass transfer, Nusselt number correlations could be used for Sherwood number calculation by replacing Pr and Ra_T with the Schmidt number, Sc , and the Rayleigh number for mass transfer, Ra_M , respectively (Bergman et al. 2017):

$$Sh = 2 + 0.56 \left(\frac{Sc Ra_M}{0.846 + Sc} \right)^{1/4} \quad (11)$$

$$Ra_M = Gr \cdot Sc \quad (12)$$

$$\text{Sh} = 2 + 0.6\text{Re}^{1/2}\text{Sc}^{1/3} \quad (13)$$

Presently, Eq. (7) and (11) were used for calculations, as stagnant droplets are considered in order to eliminate the effect of forced convection on evaporation rate. It is important to note that if $\text{Gr} \rightarrow 0$ or $\text{Re} \rightarrow 0$, the effect of natural convection for stagnant or forced convection of moving droplets is negligible, hence $\text{Nu}_0 \rightarrow 2$ and $\text{Sh} \rightarrow 2$. The enhanced convective transfer rate caused by droplet motion relative to the ambient gas is considered by Abramzon and Sirignano by introducing correction factors to Nusselt and Sherwood numbers (Abramzon and Sirignano 1989). However, these corrections in modelling are indistinguishable in the majority of practical applications (Sazhin 2014). The mass flow rate of evaporation, including the effect of Stefan flow is given by Eq. (14):

$$\dot{m}_d = \text{Sh}\pi d D_{v,a} \rho_g \ln(1 + B_M) \quad (14)$$

where the overdot notes the time derivative. Hence, the heat balance of the droplet is:

$$m_d c_{p,l} \frac{dT_s}{dt} = -h_d d^2 \pi (T_s - T_\infty) - \dot{m}_d L \quad (15)$$

where m_d is the mass of the droplet, $c_{p,l}$ is the liquid-phase specific heat capacity, h_d is the droplet heat transfer coefficient, calculated from Nu . L is the latent heat of vaporization, calculated by the Watson equation (Poling et al. 2001). The reference temperature, T_{ref} , and mass fraction of the vapor, $Y_{v,ref}$, is generally defined by the film theory (Lefebvre and McDonnell 2017; Sazhin 2014), as shown by Eqs. (16) and (17):

$$T_{ref} = T_s + \frac{T_\infty - T_s}{3} \quad (16)$$

$$Y_{v,ref} = Y_{v,s} + \frac{Y_{v,\infty} - Y_{v,s}}{3} \quad (17)$$

The gas-phase and mixture properties are calculated for these reference quantities according to the appropriate mixing rules considering fuel vapor and air (Lefebvre and McDonnell 2017):

$$c_{p,g} = Y_{v,ref} c_{p,v} + (1 - Y_{v,ref}) c_{p,a} \quad (18)$$

$$k_g = Y_{v,ref} k_v + (1 - Y_{v,ref}) k_a \quad (19)$$

$$\mu_g = Y_{v,ref} \mu_v + (1 - Y_{v,ref}) \mu_a \quad (20)$$

$$\rho_g = \left(\frac{Y_{v,ref}}{\rho_v} + \frac{1 - Y_{v,ref}}{\rho_a} \right)^{-1} \quad (21)$$

where k_v , μ_v , and ρ_v are the thermal conductivity, dynamic viscosity, and density of vapor, respectively. $c_{p,a}$, k_a , μ_a , and ρ_a are the specific heat capacity, thermal conductivity, dynamic viscosity, and density of air, respectively. Note that Eqs. (18)–(21) are limited to ideal mixture conditions when Dalton's law and Amagat's law are valid. It is also assumed that the compressibility factor is nearly unity, and the conditions are far from critical. Otherwise, a

proper equation of state (Lopez-Echeverry et al. 2017) with parameters averaged from the pure components or estimation methods with corrections for high pressure (Poling et al. 2001) should be applied to determine the properties of the gaseous medium. The justification of the application of Eqs. (18)–(21) is presented in Sect. 3. Liquid-phase properties are calculated for T_s .

After a transient heat-up period, the droplet reaches steady-state evaporation, therefore T_s remains constant, and the temporal d^2 -profile shows a linear decrease according to the d^2 -law, as shown by Fig. 1. The steady-state evaporation rate, λ_{st} , is obtained by fitting a line to the $0.15 \leq (d/d_0)^2 \leq 0.5$ data points, where d_0 is the initial droplet diameter. The slope is the λ_{st} , also applied for single droplet evaporation measurements (Nomura et al. 2017). Liquid preheating shortens the heat-up period, making λ_{st} suitable to droplet lifetime approximation.

If the temporal evolution of droplet lifetime is out of interest, and the main objective is only determining the steady-state evaporation rate, e.g. for generating a lookup table for numerical analysis, another method can be applied, as well. The other method for obtaining λ_{st} is the following. The Spalding heat transfer number can be calculated by Eq. (22):

$$B_T = \frac{c_{p,v}(T_\infty - T_s)}{L - |\dot{Q}_d|/\dot{m}_d} \quad (22)$$

where $\dot{Q}_d$ is the heat rate spent on raising the temperature of the droplet. In steady-state, it becomes zero, therefore the Spalding heat transfer number is calculated by Eq. (23):

$$B_T = \frac{c_{p,v}(T_\infty - T_s)}{L} \quad (23)$$

defining the ratio of specific heat available for droplet evaporation to the latent heat of vaporization. As T_s is constant in the steady-state evaporation phase, evaporation can be calculated by solving Eqs. (2), (3), and (23), and obtaining the steady-state droplet surface temperature, $T_{s,st}$, iteratively. Once the steady-state surface temperature is determined, all the other properties can be calculated. Even though the method has limitations, it gives a reasonably good estimation for practical applications (Lefebvre and McDonell 2017). According to the d^2 -law, the temporal variation of the squared droplet diameter is linear, and the slope is the steady-state evaporation rate, according to Eq. (24):

Fig. 1 Obtaining the steady-state evaporation rate from the temporal d^2 -profile of the droplet

$$\frac{d(d^2)}{dt} = \lambda_{st} \quad (24)$$

Considering the instantaneous mass of the fuel droplet and taking its temporal derivative, the mass flow rate can be obtained, equal to the mass flow rate of vapor at the droplet surface, using Eq. (14). Finally, the steady-state evaporation rate can be written as:

$$\lambda_{st} = \frac{4ShD_{v,a}\rho_g \ln(1 + B_M)}{\rho_l} \quad (25)$$

where ρ_l is the droplet density. If $Sh \rightarrow 2$, Eq. (25) can be simplified into:

$$\lambda_{st} = \frac{8D_{v,a}\rho_g \ln(1 + B_M)}{\rho_l} \quad (26)$$

Equation (26) ignores the effect of convection on droplet evaporation and shows that the steady-state evaporation rate depends only on the fuel material properties. However, heat and mass transfer, hence, the evaporation rate depend on Nu and Sh via Gr in the transient model, as shown by Eqs. (7)–(9) and Eqs. (11)–(12). This contradiction will be resolved in Sect. 3.

2.2 Properties of the Investigated n-alkanes

The dependence of λ_{st} on pressure and temperature was evaluated for eleven different n-alkanes, widely used in combustion systems. Also, they can be used as surrogate components of real mixtures. The pressure- and temperature-dependent material properties along with critical and boiling points are obtained from the National Institute of Standards and Technology (NIST) database (Lemmon et al. 2019). The mentioned material properties are thermal conductivity and dynamic viscosity of fuel vapor, specific heat capacity and density of liquid-phase and vapor-phase, vapor pressure, and latent heat of vaporization. The binary diffusion coefficient of vapor and air was calculated by using the method of Fuller (Fuller et al. 1966,1969). Table 1 summarizes the critical parameters, boiling temperature

Table 1 Boiling points, critical parameters, and molar masses of the investigated n-alkanes (Lemmon et al. 2019)

Name	Formula	p_c [bar]	T_c [K]	T_{bn} [K]	M_v [kg/kmol]
Methane	CH ₄	45.99	190.6	111.7	16.04
Ethane	C ₂ H ₆	48.72	305.3	184.6	30.07
Propane	C ₃ H ₈	42.48	369.8	231.1	44.10
Butane	C ₄ H ₁₀	37.96	425.1	272.7	58.12
Pentane	C ₅ H ₁₂	33.70	469.7	309.2	72.15
Hexane	C ₆ H ₁₄	30.34	507.8	341.9	86.18
Heptane	C ₇ H ₁₆	27.36	540.1	371.5	100.2
Octane	C ₈ H ₁₈	24.97	569.3	398.8	114.2
Nonane	C ₉ H ₂₀	22.81	594.6	423.9	128.3
Decane	C ₁₀ H ₂₂	21.03	617.7	447.3	142.3
Dodecane	C ₁₂ H ₂₆	18.17	658.1	489.3	170.3

at atmospheric pressure, and molar masses of the investigated n-alkanes. Undecane is missing due to the lack of data in the NIST database.

In order to get into non-dimensional space and evaluate the characteristics of different fluids in general, the temperature and pressure were defined as reduced values, i.e., the ratio of the ambient to critical values:

$$p_r = \frac{p_\infty}{p_c} \quad (27)$$

$$T_r = \frac{T_\infty}{T_c} \quad (28)$$

The general concept of using reduced values comes from the law of corresponding states (LCS), where dimensionless properties of different substances follow universal variations of dimensionless state variables, thus functions related to reduced values are similar for all substances (Poling et al. 2001). According to the limits of the investigation, the pressure range was $0.02 \leq p_r \leq 0.5$, and the temperature range was $1.2 \leq T_r \leq 1.5$, which are typical in practical combustion systems. Nonane was an exception since no data was available for $T_r > 1.3$. Note that applying the same reduced ambient conditions for the different n-alkanes results in different absolute ambient conditions as the critical parameters are unique for each substance.

3 Results and Discussions

Equation (26) in the steady-state model does not consider the effect of droplet diameter on the evaporation rate, therefore λ_{st} is independent of d . However, Nu and Sh explicitly depend on d via Gr for stagnant, and via Re for moving droplets. Consequently, λ_{st} has an indirect droplet size dependence. Figure 2a shows the deviation in λ_{st} of the transient model from the value calculated by Eq. (26) of the steady-state model. The temporal variation of Sh during the droplet lifetime for different initial droplet diameters is shown in Fig. 2b.

Fig. 2 **a** Relative deviation between the transient and steady-state models and **b** evolution of Sherwood number for different initial n-heptane droplet diameters

$t_{d_{15\%}}^2$ is the time elapsed until d^2 reduces to 15% of d_0^2 . For stagnant droplets, $Gr \rightarrow 0$, if $d \rightarrow 0$, therefore $Nu_0 \rightarrow 2$ and $Sh \rightarrow 2$ according to Eqs. (7) and (11), respectively. Thus, λ_{st} is practically independent of the diameter of small droplets, hence the difference between the transient and steady-state models can be neglected, λ_{st} is only the function of the thermophysical properties of the substance.

In Fig. 2a, the deviation is about 1% for a droplet with $d_0 = 5 \mu\text{m}$, which is representative of modern atomizers in combustion systems (Urbán et al. 2019,2017), requested indirectly by the pollutant emission standards (Directive (EU) 2015). Sh reaches a steady-state value for small droplets, and the influence of droplet diameter decreases, as shown by Fig. 2b. Therefore, the steady-state model can be used for spray calculations for tiny droplets. However, the theoretical value of λ_{st} can be corrected by Nu or Sh to consider the effect of natural or forced convection (Lefebvre and McDonell 2017).

The deviation between the two models can be neglected for fine droplets, hence the transient model converges to the steady-state model at various conditions, as shown by Fig. 3. Figure 4 presents the decreasing Lewis number during the heat-up period as the initial evaporating mass is small. However, it remains above unity for steady-state evaporation, therefore, the $Le = 1$ assumption (Lefebvre and McDonell 2017) may lead to significant bias.

Fig. 3 The convergence of the transient model to the steady-state model for droplet surface temperature in the case of a single evaporating $5 \mu\text{m}$ n-heptane droplet

Fig. 4 Temporal evolution of Lewis number

The calculated steady-state properties influencing evaporation are discussed next for different reduced pressure and temperature conditions. All the trends correspond to steady-state, which characterizes vaporization at a given condition. Properties of n-butane and n-octane are discussed together to show the effect of molar mass and carbon chain length. Note that T_s is increasing with both pressure and temperature, as shown by Fig. 3, leading to increased vapor-air film temperature around the droplet. For all the investigated vapor-air mixtures, the compressibility factor was between 0.95 and 1. The lower values correspond to high pressure and low temperature. Consequently, the ideal gas assumption in Eq. (1) and the ideal mixture model in Eqs. (18)–(21) are appropriate for the present work.

Figure 5 shows that Le notably exceeds unity at low pressure and temperature, which is relevant for steady-operating combustion systems, such as boilers, furnaces, and gas turbines. $c_{p,v}/c_{p,g}$, divided by Le in the exponent of B_T in Eq. (3), is shown by Fig. 6. Elevated pressure increases $c_{p,v}$, which is more significant at lower temperatures, near the critical point. The decrease of Le and increase of specific heat capacity ratio enhance each other at higher pressure, increasing the exponent of Eq. (3), as shown by Fig. 7. Therefore, the unity exponent of Eq. (3) may lead to significant bias in droplet evaporation calculations.

Fig. 5 Le of **a** n-butane and **b** n-octane at various ambient conditions

Fig. 6 The ratio of vapor specific heat capacity to mixture specific heat capacity of **a** n-butane and **b** n-octane

Fig. 7 The exponent of Eq. (3) for **a** n-butane and **b** n-octane

Figure 8 shows that B_T increases with both pressure and temperature, while Fig. 9 shows that the specific heat available for droplet vaporization has a minimum at low T_r and monotonously decreasing at high T_r with p_r . The difference between T_∞ and $T_{s,st}$ decreases with increasing p_r , since the steady-state droplet surface temperature is higher at higher pressure. On the other hand, increasing T_r , thus T_∞ increases the difference. $c_{p,v}$ increases with p_r , especially at lower temperatures, resulting in a small increase in the specific heat at low temperatures. However, at high temperatures, the decrease in the temperature difference dominates the trends. L decreases with both p_r and T_r , resulting in an overall increase in B_T with pressure.

The different terms of Eq. (26) are evaluated next in order to characterize the trends of steady-state evaporation rate. The binary diffusion coefficient of vapor and air decreases with pressure and increases with temperature, as shown by Eq. (5). However, increasing pressure also increases the temperature of the gaseous mixture around the droplet. The density of the vapor-air mixture increases with pressure and decreases with temperature. Increasing pressure or temperature decreases droplet density as the

Fig. 8 Variation of Spalding heat transfer number of **a** n-butane and **b** n-octane

Fig. 9 Available specific heat for droplet evaporation for **a** n-butane and **b** n-octane

temperature of the droplet increases. Higher pressure enhances this effect, thus the decrease of ρ_l with temperature is more significant at higher pressures.

Figure 10 shows the term $D_{v,a} \cdot \rho_g / \rho_l$ from Eq. (26) for C_2 – C_9 n-alkanes, where the trends are matching for the different molecules, except for ethane. However, ethane has a

Fig. 10 The term $D_{v,a} \cdot \rho_g / \rho_l$ from Eq. (26) for C_2 – C_9 n-alkanes for different temperatures

slightly different molecular structure as it has only two CH_3 groups without a CH_2 group. Nevertheless, this difference shrinks as temperature increases. This behavior of ethane was highlighted by Ewender and Welle (Ewender and Welle 2019). They experimentally investigated the permeation and diffusion characteristics of n-alkanes from methane up to n-dodecane through a polyethylene naphthalate film since their focus was on the barrier properties of polymers. The diffusion coefficients of methane and ethane were reported slightly outlying, referring to the different molecular structures (see Fig. 4 in ref. (Ewender and Welle 2019)).

Figure 11 shows the trends of B_M , which decreases at low and increases at high temperatures with pressure. At moderate temperature, B_M is independent of pressure. The same trends can be observed for $Y_{v,s}$ and $p_{v,s}/p_\infty$, resulting from Eq. (1). $p_{v,s}$ increases with increasing ambient pressure as the droplet surface temperature increases, however, the increase is more significant at higher temperatures as that temperature range is characterized by the upper part of the vapor pressure curve, as shown by Fig. 12.

Figure 13 shows the variation of λ_{st} . The diverging trends of ρ_l and B_M for different temperatures lead to a diverging trend in λ_{st} as well, therefore increasing p_r has a more significant

Fig. 11 Variation of Spalding mass transfer number for **a** n-butane and **b** n-octane

Fig. 12 Vapor pressure versus surface temperature of the droplet for n-butane and n-octane

Fig. 13 Steady-state evaporation rate for n-butane (**a**) and n-octane (**b**)

effect at higher T_r . This behavior is more obvious by introducing the non-dimensional steady-state evaporation rate, Λ_{st} , which is the ratio of the pressure-dependent steady-state evaporation rate to the steady-state evaporation rate at 1 bar ambient pressure and the same ambient temperature, defined by Eq. (29):

$$\Lambda_{st}(p_r, T_r) = \frac{\lambda_{st}(p_r, T_r)}{\lambda_{st,1\text{bar}}(T_r)} \quad (29)$$

Figure 14 shows the trends of Λ_{st} . Saturation can be observed at lower T_r , therefore, further increasing p_r leads to only a slight enhancement of droplet vaporization. On the other hand, increasing pressure at high ambient temperature notably improves evaporation.

Figure 15 shows that Λ_{st} of C_2 – C_9 n-alkanes is similar in the range of $1.3 \leq T_r \leq 1.5$, allowing curve fitting by using LCS for calculating λ_{st} . Power function in the form of $\Lambda_{st} = a(T_r) \cdot p_r^b + c$ gave a satisfactory fit. $a(T_r)$ and $b(T_r)$ functions both took a similar form, $\alpha \cdot T_r^\beta + \gamma$, leading to Eq. (30):

Fig. 14 Non-dimensional steady-state evaporation rate for **a** n-butane and **b** n-octane

Fig. 15 Non-dimensional steady-state evaporation rate for C_2 – C_9 n-alkanes at various ambient temperatures

$$\Lambda_{st} = [-1.279T_r^{-1.7202} + 1.279]p_r^{-0.5214T_r^{-3.191}+0.7626} + 0.9325 \quad (30)$$

The validity of Eq. (30) is $0.02 \leq p_r \leq 0.5$, $1.3 \leq T_r \leq 1.5$, and n-alkanes of C_2 – C_9 . The parameters of the curve fitting can be found in "Appendix 2". The uncertainty of the present model is discussed in "Appendix 3", considering the uncertainty of the material data, including cross-sensitivity.

With Eq. (30), the steady-state non-dimensional evaporation rate can be calculated with two parameters, T_c and p_c . Thus, given the atmospheric evaporation characteristics, the steady-state evaporation rate of the droplet can be obtained for a given pressure and temperature in the validity range. As forced convection enhances vaporization, the calculated evaporation rate can be corrected by Re with a proper Nu and Sh correction factor (Lefebvre and McDonell 2017; Sazhin 2014), thus Eq. (30) is applicable for spray calculations in general.

4 Conclusions

The effect of ambient pressure and temperature on the characteristics of the steady-state evaporation rate of eleven different n-alkane droplets has been investigated by comparing the versatile steady-state d^2 -law with a transient evaporation model used in the

state-of-the-art numerical codes. The material properties of the fluids were acquired from the NIST database. The range of pressure and temperature was defined as reduced values by using the critical properties. Based on the results, the following conclusions were derived:

1. For small droplets ($d_0 \approx 5\text{--}10\ \mu\text{m}$), the deviation between steady-state and transient models can be neglected. In this case, Nu and Sh are practically independent of droplet size, therefore the steady-state evaporation rate only depends on the thermophysical properties of the fluid.
2. Lewis number notably exceeds unity during the transient heat-up period and remains above one for the steady-state evaporation for the investigated n-alkanes. Higher values correspond to low pressure and low temperature. Consequently, revising the Lewis number, even in a simple case, is highly recommended to avoid a notable bias.
3. The ratio of vapor specific heat capacity to mixture specific heat capacity increases with pressure and decreases with temperature, like $c_{p,v}$ significantly rises with pressure closer to the critical temperature.
4. The trends of term $D_{v,a} \cdot \rho_g / \rho_l$ from Eq. (26) for $C_2\text{--}C_9$ n-alkanes are practically identical, however ethane shows a larger deviation at low temperature. This decreases with increasing the ambient temperature.
5. B_M decreases at low temperature and increases at high temperature with pressure, because of $p_{v,s}/p_\infty$ increases at high, and decreases at low temperatures with pressure.
6. λ_{st} increases with pressure, however the increase is more significant at higher temperatures due to the enhanced increment in $p_{v,s}/p_\infty$ and the decrease in ρ_l .
7. The non-dimensional evaporation rate, Λ_{st} , is practically identical for $C_2\text{--}C_9$ n-alkanes at $0.02 \leq p_r \leq 0.5$, $1.3 \leq T_r \leq 1.5$, allowing to apply a two-parameter corresponding states method by using Eq. (30).

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Compliance with Ethical Standards

Conflict of interest The authors declare that there is no conflict of interest.

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Appendix 1: Validation of the Evaporation Model

The present results are validated against ref. (Chung and Kawaguchi 1995) where the evaporation of $d_0=200\text{ }\mu\text{m}$ n-heptane droplets is investigated using a drop tower. The velocity of the droplets and the air stream are almost equal, thus the reported value of Re is 0.3. Figure 16 shows the comparison between the free-falling droplet measurement data and calculation. A correction factor was introduced in order to consider forced convection, therefore the calculated steady-state evaporation rate values were multiplied by a factor of $(1+0.3Re^{1/2}Sc^{1/3})$ according to the Sh correction (Lefebvre and McDonell 2017). Calculated λ_{st} values show a good agreement with measurement data. Only a small discrepancy can be observed. Note that model validation with suspended droplet measurements is more challenging and requires special attention as the heat balance of the droplet is notably affected by the support fiber, resulting in an enhanced vaporization rate (Yang and Wong 2001,2002; Chauveau et al. 2019). Presently, no experimental data was used from this latter measurement type.

Fig. 16 Validation of the evaporation model for free-falling n-heptane droplets

Appendix 2: Curve Fitting Parameters of the Non-Dimensional Steady-State Evaporation Rate

Tables 2 and 3 contain the parameters of the curve fitting of Eq. (30). These parameters are the a , b , c , α , β , and γ coefficients and their upper and lower confidence bounds ($cb+$ and $cb-$ respectively).

Table 2 Parameters of the curve fitting for Eq. (30) I

T_r	1.3	1.35	1.4	1.45	1.5
a	0.4647	0.5150	0.5621	0.6043	0.6419
b	0.5376	0.5610	0.5851	0.6041	0.6192
c	0.9325	0.9325	0.9325	0.9325	0.9325
a_{cb-}	0.4585	0.5095	0.5566	0.5977	0.6333
b_{cb-}	0.5273	0.5528	0.5774	0.5954	0.6085
a_{cb+}	0.4709	0.5204	0.5676	0.6110	0.6505
b_{cb+}	0.5478	0.5693	0.5928	0.6128	0.6299
SSE	0.007385	0.004167	0.003896	0.005386	0.008577
R^2	0.9905	0.9951	0.9962	0.9954	0.9936
DFE	158	138	138	138	138
Adjusted R^2	0.9904	0.9951	0.9962	0.9954	0.9935
$RMSE$	0.006837	0.005495	0.005313	0.006247	0.007884

Table 3 Parameters of the curve fitting for Eq. (30) II

	a	b
α	-1.279	-0.5214
β	-1.7202	-3.191
γ	1.279	0.7626
α_{cb-}	-1.568	-0.5795
β_{cb-}	-2.618	-7.5600
γ_{cb-}	0.9022	0.5146
α_{cb+}	-0.9903	-0.4634
β_{cb+}	-0.8225	1.177
γ_{cb+}	1.656	1.011
SSE	7.662E-07	3.886E-06
R^2	1.000	0.9991
DFE	2	2
Adjusted R^2	0.9999	0.9982
$RMSE$	0.006189	0.001394

Appendix 3: Uncertainty Analysis of Λ_{st}

Table 4 summarizes the relative uncertainty of each material property for the different n-alkanes. Note that the binary diffusion coefficient is calculated with Eq. (5), thus uncertainty values corresponding to $D_{v,a}$ refer to measurement data of n-alkane-nitrogen systems from ref. (Winkelmann 2007), as no uncertainty data was available for the method of Fuller. Air composition was 21 V/V% O₂ and 79 V/V% N₂. Λ_{st} is the ratio of the steady-state evaporation rate to the steady-state evaporation rate at 1 bar ambient pressure. According to Eq. (29), the corresponding material properties (e.g., vapor density at a given pressure and 1 bar) in the numerator and denominator are correlated, resulting in a final reduction of the deviation of Λ_{st} due to the cross-correlation terms, which were assumed to be unity for the identical material properties. Consequently, the data uncertainty can be lower than the uncertainty of each value if they are correlated as long as the sign of the cross derivatives multiplied by the correlation of the two quantities is negative. The deviation of Λ_{st} was determined by Eq. (31) (Coleman and Steele 2018):

$$\sigma_{\Lambda_{st}} = \sqrt{\sum_{i,j} \left(\frac{\partial \Lambda_{st}}{\partial x_i} \cdot \frac{\partial \Lambda_{st}}{\partial x_j} \cdot \sigma_{x_i} \cdot \sigma_{x_j} \cdot \text{corr}(x_i, x_j) \right)} \quad (31)$$

where $\text{corr}(x_i, x_j) = 1$, when $i = j$ or x_i and x_j are identical variables, otherwise $\text{corr}(x_i, x_j) = 0$. The values of the relative error are shown by Fig. 17 for C₂–C₉ n-alkanes, which are well below 1% for all the investigated conditions, because of the very low relative uncertainty of vapor-phase and liquid-phase densities, and the correlated quantities.

Table 4 The relative uncertainty of material properties of the investigated n-alkanes obtained from the NIST database (Lemmon et al. 2019) and ref. (Winkelmann 2007)

Name	$\sigma\rho/\rho$ [%]	$\sigma c_p/c_p$ [%]	$\sigma k_v/k_v$ [%]	$\sigma\mu/\mu_v$ [%]	$\sigma p_{v,s}/p_{v,s}$ [%]	$\sigma D_{v,a}/D_{v,a}$ [%]
Methane	0.07	1	2.5	2	0.5*	2
Ethane	0.2	2.5	2	2	0.5*	2
Propane	1*	5*	5	4	0.5*	2
Butane	1	5	5	3	1.5	2
Pentane	0.5	2	5*	5*	0.2	2
Hexane	0.5	2	5*	5*	0.2	2
Heptane	0.5	2	5*	5*	0.2	2
Octane	0.5	2	5	5	0.2	2
Nonane	1	5	5	5	0.5	2
Decane	2	1	5	5	0.2	2
Dodecane	0.5	1	5	5	5	2
Air	0.1	2	2	2	–	–

*No data was available on uncertainty, thus the values were chosen to be similar to the neighboring data

Fig. 17 The relative error of non-dimensional steady-state evaporation rate for C_2 – C_9 n-alkanes

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