

## THE EFFECT OF TEMPERATURE DEPENDENCE OF DENSITY AND MASS DIFFUSION COEFFICIENT ON THE MASS TRANSPORT FROM A DROP EVAPORATING IN HOT GASEOUS ENVIRONMENT

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### ABSTRACT

Species, energy and momentum conservation equations are solved in spherical symmetry and under ideal gas approximation, to yield an analytical model capable to evaluate the heat transfer and the evaporation rate from a drop under quasi-steady conditions, accounting for the temperature dependence of mixture density and diffusion coefficient. The model is applied to predict the evaporation rate from water and hydrocarbon droplets under pressure and temperature conditions of interest for applicative fields, like fire control and combustion. The results obtained by the proposed model are compared with those from the most commonly used ones where mass diffusion coefficient and gas density are kept constant to an average value.

### INTRODUCTION

Drop evaporation in a hot gaseous environment is of fundamental importance for a wide range of engineering applications, like in spray combustion, spray cooling, spray drying, fire suppression, etc. The evaporation process involves simultaneous heat and mass transfer and a wide literature is available on the modelling of the complex physical phenomena involved (see [1] for a thorough review). To numerically simulate evaporating spray using CFD methodologies, detailed models based on single drop analysis have to be simplified to be CPU efficient and this forced the introduction of many simplifying hypotheses to develop the nowadays available evaporation models. Constant properties of the gas mixture, quasi-steadiness, drop sphericity are among the most common approximations, and the most frequently used models (see for example [2]) are based on these assumptions, although recently, attempts to relieve some of them became available in the open literature [3-4].

Modelling of mass transfer and thermal phenomena occurring within the liquid phase in an evaporating drop has been object of deep investigation and an extensive literature became available in the latest years (see [1,5] for reference). The most simplified models, used in many conventional CFD codes for spray applications, assume infinite liquid thermal conductivity when modelling the drop heating, neglecting

temperature gradient inside the drop [5]. There exists experimental evidence [6,7] that contradicts this assumption and to cope with these findings this issue has been addressed introducing a finite effective thermal conductivity, which takes into account also the effect of liquid recirculation inside the drop [1,5]. The totality of the analytical evaporation models implemented in commercial CFD codes neglects moving boundary effect due to radius shrinking; this hypothesis has been removed by Sazhin *et al.* in [8,9], who included the effect of a moving boundary to solve the conservation equations in the liquid phase. The comparison with previous models shows that drop shrinking has a non neglectful effect on liquid temperature prediction, yielding longer evaporation times compared to the conventional approach and reaffirming that such effect cannot be ignored when accurate predictions are needed.

When a drop is injected into a hot gas, large temperature gradients are achieved and the previously mentioned constant property approximation becomes questionable since at least gas density and diffusion coefficient have a strong dependence on temperature. The use of an average value for all those properties that are expected to significantly change with temperature, commonly obtained by the '1/3-rd rule' [10], may not be enough to correctly catch the main features of the phenomenon. Recently it was shown that a model that takes into account gas temperature and density gradient effects may yield significant differences respect to the classical ones, and it may better perform when compared with available experimental results obtained under high gas temperature conditions [3]. Among other parameters, the diffusion coefficient of a vapour in a gaseous mixture shows a significant temperature dependence, statistical thermodynamics [11] predicts a power law dependence on the absolute temperature with exponent equal to 3/2, while the widely used Fueller-Scheller-Giddings correlation [12] suggests a value of 7/4 for the same exponent.

Numerical models for drop evaporation studies have been deeply refined over the decades including more complex physical aspects like drop composition, shape, interaction with other drops and/or solid surfaces (see [13,14] for reference) and obviously also detailed model to evaluate the temperature

dependence of all the involved thermo-physical properties. However, due to the complexity of the numerical implementation and the CPU time required for a single drop test case simulation, they can be used only as benchmarking for simpler models to be developed.

The main aim of this work is to develop an evaporation model for single component drops that includes the effect of gas density and diffusion coefficient temperature variation, with the target to efficiently implement it in comprehensive CFD tools for sprays injected in hot environment.

## NOMENCLATURE

Roman symbols

$c_p$	[J/kgK]	Specific heat at constant pressure
$c$	[kmol/m <sup>3</sup> ]	Molar density
$D_{10}$	[m <sup>2</sup> /s]	Binary diffusion coefficient
$F$	[-]	Function, equation (14)
$G$	[-]	Logarithm of gas mass fraction
$k$	[W/mK]	Thermal conductivity
$K_0$	[-]	Coefficient, equation (11)
$Le$	[-]	Lewis number
$Le^M$	[-]	Modified Lewis number
$m_{ev}$	[kg/s]	Mass evaporation rate
$Mm$	[kg/kmol]	Molar mass
$n$	[-]	Exponent, equation (9)
$P_T$	[Pa]	Pressure
$r$	[m]	Radial coordinate
$R$	[J/kmolK]	Universal gas constant
$R_0$	[m]	Drop radius
$Sc$	[-]	Schmidt number
$T$	[K]	Temperature
$U$	[m/s]	Stefan velocity
$y$	[-]	Molar fraction
$Y$	[-]	Non-dimensional evaporation rate

Greek symbols

$\chi$	[-]	Mass fraction
$\rho$	[kg/m <sup>3</sup> ]	Mass density
$\Lambda$	[-]	Non-dimensional number (equation 6a)
$\theta$	[-]	Molar mass ratio
$\zeta$	[-]	Non-dimensional radial coordinate, $\zeta=R_0/r$
$\Psi$	[-]	Evaporation rate ratio

Subscripts

$r$	Radial component
$ref$	Reference condition
$s$	Surface
$\infty$	Free stream condition
$0$	Ambient or reference

Superscripts

$c$	Constant mass density
(0)	Gas
(1)	Vapour
$\sim$ ^	Non-dimensional

Abbreviations

CFD	Computational Fluid Dynamics
CPU	Central Processing Unit
ODE	Ordinary Differential Equation

## MODEL EQUATIONS

The species conservation equations for a single component spherical drop steadily evaporating in a hot gaseous environment can be written in simplified form as follows (see [15] and also [3] for further details):

$$\rho U \chi^{(0)} - \rho D_{10} \frac{d\chi^{(0)}}{dr} = 0 \quad (1a)$$

$$\rho U \chi^{(1)} - \rho D_{10} \frac{d\chi^{(1)}}{dr} = \frac{m_{ev}}{4\pi r^2} \quad (1b)$$

where, due to the assumption of a stationary liquid-gas interface,  $m_{ev}$  is the actual evaporation rate (refer to the nomenclature for the meaning of the other symbols) and the gas flux is nil everywhere (see again [15]). Summation of the two equations yields the mass conservation equation:

$$\rho U = \frac{m_{ev}}{4\pi r^2} \quad (2)$$

The momentum and the energy conservation equations for the evaporating drop in spherical symmetry, under the same simplifying hypotheses as in [3], are:

$$\rho U \frac{dU}{dr} = -\frac{dP_T}{dr} + \mu \left( \frac{d^2U}{dr^2} + \frac{2}{r} \frac{dU}{dr} \right) \quad (3a)$$

$$\rho U c_p \frac{dT}{dr} = k \left( \frac{d^2T}{dr^2} + \frac{2}{r} \frac{dT}{dr} \right) \quad (3)$$

The usual approach to the problem is to define some reference conditions to which evaluate the average value of the fluid properties; in particular the gaseous mixture density  $\rho$  and the binary diffusion coefficient  $D_{10}$  depends on temperature and the '1/3-rd rule' is usually applied to define the reference temperature [10]:

$$T_{ref} = \frac{2T_s + T_\infty}{3} \quad (4)$$

and  $\rho_{ref} = \rho(T_{ref})$ ,  $D_{10,ref} = D_{10}(T_{ref})$ . Considering that  $\chi^{(1)} + \chi^{(0)} = 1$ , the second species equation (1b) can be obtained from equations (1a) and (2) and introducing the following non-dimensional variables:

$$\zeta = \frac{R_0}{r}; \quad G = \ln(\chi^{(0)}); \quad \tilde{T} = \frac{T}{T_\infty}; \quad \tilde{\rho} = \frac{\rho}{\rho_\infty}; \quad \tilde{D}_{10} = \frac{D_{10}}{D_{10,ref}} \quad (5)$$

and the parameters:

$$Y = \frac{m_{ev} c_{p,ref}}{4\pi R_0 k_{ref}}; \quad \Lambda = \frac{RT_\infty R_0^2}{Mm^{(1)} D_{10,ref}^2} \quad (6a)$$

$$Le = \frac{k_{ref}}{\rho_\infty c_{p,ref} D_{10,ref}}; \quad \hat{P}_T = \frac{P_T Mm^{(1)}}{RT_\infty \rho_\infty} \quad (6b)$$

the above reported species, momentum and energy conservation equations reduce to:

$$\tilde{D}_{10} \tilde{\rho} \frac{dG}{d\zeta} = -YLe \quad (7a)$$

$$-\frac{d\hat{P}_T}{d\zeta} = \frac{\zeta^2}{\Lambda} \left( Sc \frac{d^2\tilde{U}}{d\zeta^2} + YLe \frac{d\tilde{U}}{d\zeta} \right) \quad (7b)$$

$$Y \frac{d\tilde{T}}{d\zeta} + \frac{d^2\tilde{T}}{d\zeta^2} = 0 \quad (7c)$$

It has already been shown [3] that, for a large variety of conditions of interest for applications, the non-dimensional parameter  $\Lambda$  assumes quite large values, then justifying the use of an asymptotic form (for  $\Lambda \rightarrow \infty$ ) of the momentum equation that in the present case simply becomes:  $dP_T/d\zeta=0$  or:

$$\hat{P}_T = \hat{P}_{T,\infty} \quad (8)$$

which, under the assumption of ideal gas behaviour for the gaseous mixture, yields:

$$(1 + \theta\chi^{(0)})\tilde{\rho}\tilde{T} = \hat{P}_{T,\infty} \quad (9)$$

where  $\theta = \frac{Mm^{(1)} - Mm^{(0)}}{Mm^{(0)}}$ .

The binary mass diffusion coefficient is expected to depend on temperature following the general rule:

$$\tilde{D}_{10} = \frac{\tilde{T}^n}{\tilde{T}_{ref}^n} \quad (10)$$

where:  $n=0$  stands for the case of constant diffusion coefficient, which is the usual assumption that yields to the classical results [16,2],  $n=3/2$  is the value suggested by classical statistical thermodynamics [11] and  $n=7/4$  is the value given by the widely used FSG correlation [12].

## BOUNDARY CONDITIONS AND ANALYTIC SOLUTIONS

The B.C. for the energy equation can be set as:

$$T(r = R_0) = T_s; \quad T(r = \infty) = T_\infty \quad (11)$$

and the well known analytic solution is:

$$\tilde{T}(\zeta) = (1 - K_0)e^{-Y\zeta} + K_0 \quad (12)$$

where  $K_0 = \frac{\tilde{T}_s - e^{-Y}}{1 - e^{-Y}}$ .

Equation (7a) can be transformed, using equations (9) and (10) into the following ODE:

$$\frac{G_\zeta}{1 + \theta e^G} = \left( -\frac{YLe\tilde{T}_{ref}^n}{1 + \theta\chi_\infty^{(0)}} \right) \tilde{T}^{1-n}(\zeta) \quad (13)$$

The analytic solution of equation (13) exists for many rational values of the parameter  $n$  (those for which the integral  $I_n(\zeta) = \int \tilde{T}^{1-n}(\zeta) d\zeta$  can be analytically evaluated). Applying the Dirichlet boundary conditions:

$$G(0) = \ln(1 - \chi_s^{(1)}); \quad G(1) = \ln(1 - \chi_\infty^{(1)}) \quad (14)$$

the following equation can be derived:

$$\frac{1 + \theta\chi_\infty^{(0)}}{Le\tilde{T}_{ref}^n} \ln \left( \frac{\chi_\infty^{(0)}(1 + \theta\chi_s^{(0)})}{\chi_s^{(0)}(1 + \theta\chi_\infty^{(0)})} \right) = F_n(K_0, \tilde{T}_s) \quad (15)$$

where the integral  $F_n = Y \int_0^1 \tilde{T}^{1-n}(\zeta) d\zeta$  can conveniently be written in terms of the parameter  $K_0$  instead of  $Y$ , since its functional form depends on the sign of  $K_0$  for  $n \neq 0$ . Noticing that:

$$\frac{\chi^{(0)}}{1 + \theta\chi^{(0)}} = \frac{1 - y^{(1)}}{1 + \theta} \quad (16)$$

where  $y^{(1)}$  is the vapour molar fraction; introducing the molar density  $c = \frac{P_r}{RT}$  and the modified Lewis number:

$$Le^M = \frac{k_{ref}}{c_{ref} Mm^{(1)} D_{10,ref} c_{p,ref}} \quad (17)$$

equation (15) can be written in a simpler form:

$$\frac{1}{Le^M \tilde{T}_{ref}^{n-1}} \ln \left( \frac{1 - y_s^{(1)}}{1 - y_\infty^{(1)}} \right) = F_n(K_0, \tilde{T}_s) \quad (18)$$

The expressions of  $F_n$  for the three values of  $n$  of interest in this analysis are reported in the following equations:

$$F_{7/4} = \begin{cases} \left. \begin{aligned} & \ln \left( \frac{\tilde{T}_s^{1/4} + K_0^{1/4} (1 - K_0^{1/4})}{\tilde{T}_s^{1/4} - K_0^{1/4} (1 + K_0^{1/4})} \right) + \\ & \frac{1}{K_0^{3/4}} \left\{ 2 \arctan \left( \frac{\tilde{T}_s^{1/4}}{K_0^{1/4}} \right) + \right. \\ & \left. - 2 \arctan \left( \frac{1}{K_0^{1/4}} \right) \right\} \end{aligned} \right\} K_0 > 0 \\ \frac{4}{3} \left( \frac{1}{\tilde{T}_s^{3/4}} - 1 \right) \quad K_0 = 0 \\ \left. \begin{aligned} & \ln \left( \frac{A_+(K_0, \tilde{T}_s) A_-(K_0, 1)}{A_-(K_0, \tilde{T}_s) A_+(K_0, 1)} \right) + \\ & \frac{-2^{-1/2}}{|K_0|^{3/4}} \left\{ 2 \arctan(B(K_0, 1)) + \right. \\ & \left. - 2 \arctan(B(K_0, \tilde{T}_s)) \right\} \end{aligned} \right\} K_0 < 0 \end{cases} \quad (19a)$$

$$A_\pm(K_0, x) = |K_0|^{1/2} \pm \sqrt{2} |K_0|^{1/4} x^{1/4} + x^{1/2}$$

$$B(K_0, x) = \frac{|K_0|^{1/2} - x^{1/2}}{\sqrt{2} |K_0|^{1/4} x^{1/4}}$$

$$F_{3/2} = \begin{cases} \frac{1}{K_0^{1/2}} \ln \left( \frac{\tilde{T}_s^{1/2} + K_0^{1/2}}{\tilde{T}_s^{1/2} - K_0^{1/2}} \frac{1 - K_0^{1/2}}{1 + K_0^{1/2}} \right) & K_0 > 0 \\ 2 \left( \frac{1}{\tilde{T}_s^{1/2}} - 1 \right) & K_0 = 0 \\ \frac{2}{|K_0|^{1/2}} \left\{ \arctan \left( \frac{1}{|K_0|^{1/2}} \right) + \right. \\ \left. - \arctan \left( \frac{\tilde{T}_s^{1/2}}{|K_0|^{1/2}} \right) \right\} & K_0 < 0 \end{cases} \quad (19b)$$

$$F_0(K_0, \tilde{T}_s) = (1 - \tilde{T}_s) + K_0 \ln \frac{K_0 - 1}{K_0 - \tilde{T}_s} \quad (19c)$$

The solution of the non-linear equation (18), using an iterative method, allows to evaluate  $K_0$  and the evaporation rate can be calculated from the definition of  $K_0(Y, \tilde{T}_s)$ :

$$m_{ev} = 4\pi R_0 \frac{k_{ref}}{c_{p,ref}} \ln \frac{K_0 - 1}{K_0 - \tilde{T}_s} \quad (20)$$

## RESULTS AND DISCUSSION

The classical model [16] is found by solving the above reported species conservation equations under the hypotheses that  $\rho$  and  $D_{10}$  are independent of temperature. In such case a reference value for these parameters is chosen, usually through the '1/3-rd rule' [10], using equation (4) for the reference temperature and the following one for the reference species mass fractions:

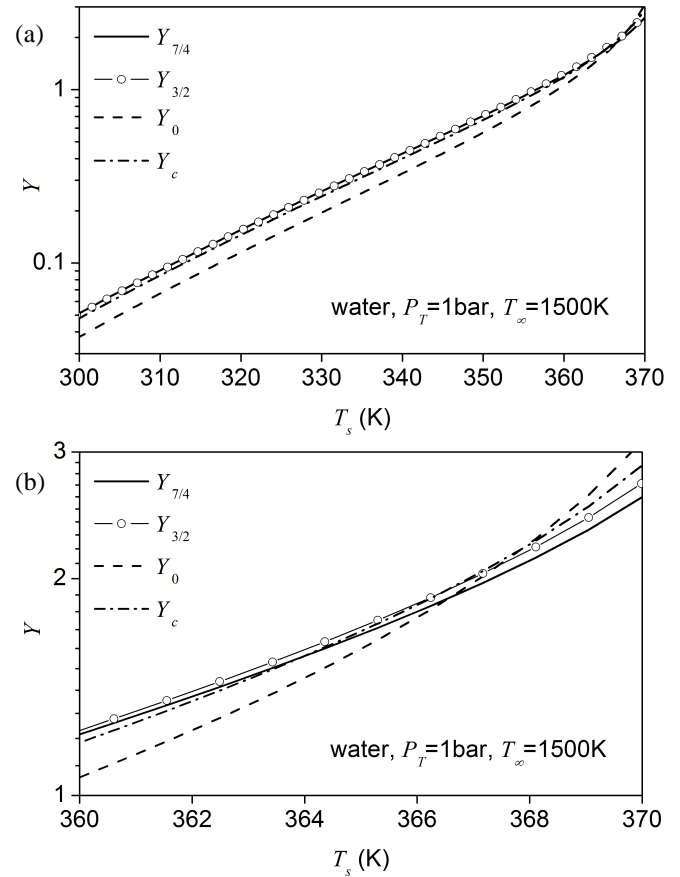
$$\chi_{ref}^{(1)} = \frac{2\chi_s^{(1)} + \chi_\infty^{(1)}}{3} \quad (21)$$

and the corresponding evaporation rate is:

$$m_{ev}^c = 4\pi R_0 \rho_{ref} D_{10ref} \ln \frac{1 - \chi_\infty^{(1)}}{1 - \chi_s^{(1)}} \quad (22)$$

The effect of temperature dependence on gaseous mixture density and diffusivity on the instantaneous drop evaporation rate is investigated using the analytical models described in the previous section (equations 19), which have been compared with the constant property model (equation 22). The comparison has been made selecting as evaporating fluid water and n-octane, which are representative of fire control and internal combustion engine spray applications. All the results presented in the following paragraphs are obtained under steady-conditions, setting  $y_\infty^{(1)} = 0$ ,  $\chi_\infty^{(1)} = 0$ .

Figure 1(a) shows the effect of liquid temperature on the non-dimensional evaporation rate  $Y$  (equation 6a) for water drop vaporising under steady condition at 1bar and 1500K gaseous environment, as predicted by the variable property models with exponent  $n=7/4$  and  $n=3/2$  (see equations 19a and 19b, respectively), by the variable density model ( $n=0$ , equation 19c) and by the constant property model (equation 22). The graph evidences that the two variable property models predict very similar results through all the selected range of operating conditions. The variable density model noticeably under-predicts the evaporation rate for drop temperature far from the boiling point. As the drop temperature increases the predictions from the variable density model approach the ones from the more complete variable property models and a small temperature window exists where all the models predict almost the same results, then the trend inverts and the variable density model over-estimates the evaporation rate predicted by the variable property models.



**Figure 1** (a) Effect of drop temperature on non-dimensional evaporation rate predicted by the four models for water drop at 1bar and 1500K; (b) zoom of (a) close to the boiling point.

This is evidenced in Figure 1(b), which shows the zoom of Figure 1(a) focusing on the temperature window close to the boiling point. The constant property model follows a similar trend of the variable density model, but the discrepancy from

the variable property models is substantially reduced. The reason for such behaviour is related to the temperature dependence of density and diffusion coefficient, which product enters in the relation defining the drop evaporation rate.

To better appreciate the comparison among the different models, the evaporation rate is reported in non-dimensional form, where the variable property model with  $n=7/4$  is taken as reference case:

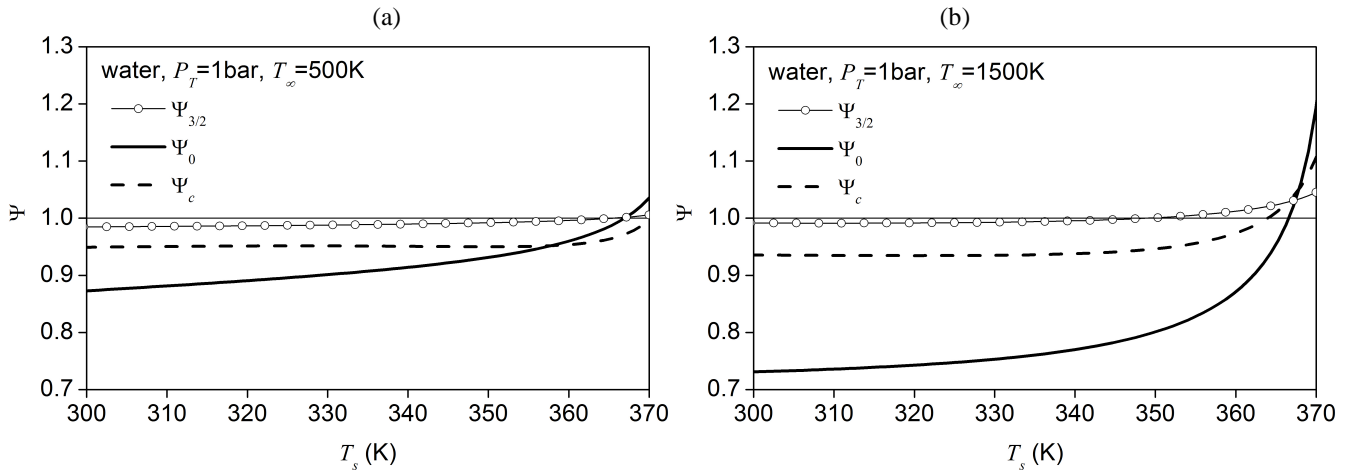
$$\Psi_* = \frac{Y_*}{Y_{7/4}} \quad (23)$$

Figure 2 shows the effect of drop temperature on the evaporation rate ratio for water drop evaporating at atmospheric pressure conditions and temperature equal to 500K and 1500K, figures (a) and (b) respectively. The results from the four models are reported showing that the two variable property models are in rather good agreement with differences up to about 5% under highly evaporating conditions. The increase of gas temperature enhances the discrepancy of the constant

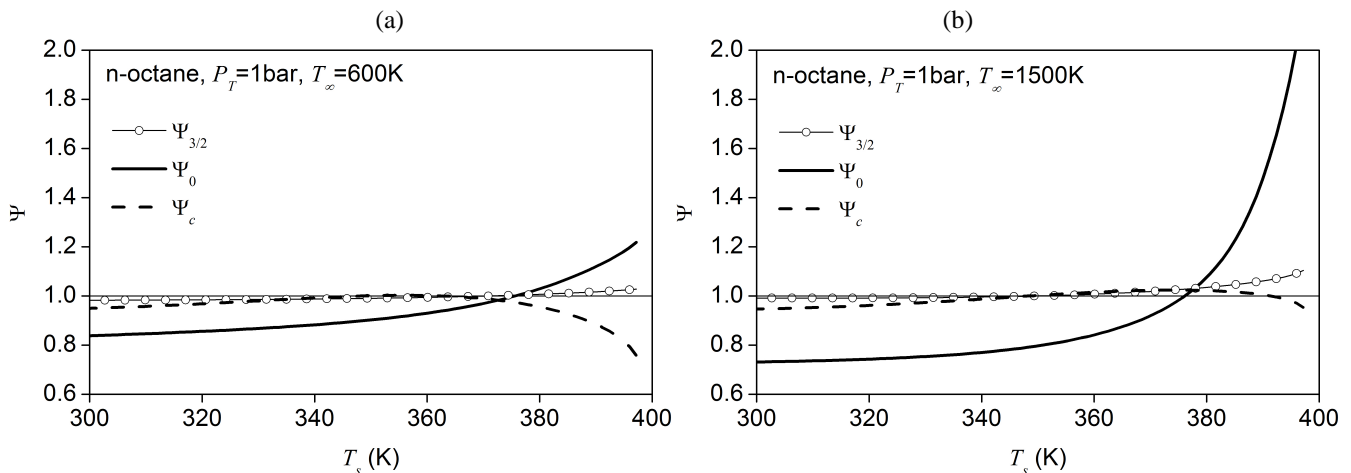
property and variable density models compared to the reference case.

Figure 3 presents the comparison of  $\Psi$  as predicted by the four models for n-octane drop at 1 bar and gas temperature equal to 600 and 1500K (figure 3a and 3b, respectively), confirming the previous outcomes with only a different behaviour predicted by the constant property model that substantially under-predicts the evaporation rate at high drop temperatures. The opposite mechanism of the constant property model in case of n-octane compared to water (see figure 2) is due to the opposite value of the parameter  $\theta$ , which is positive in case of hydrocarbons and negative for water.

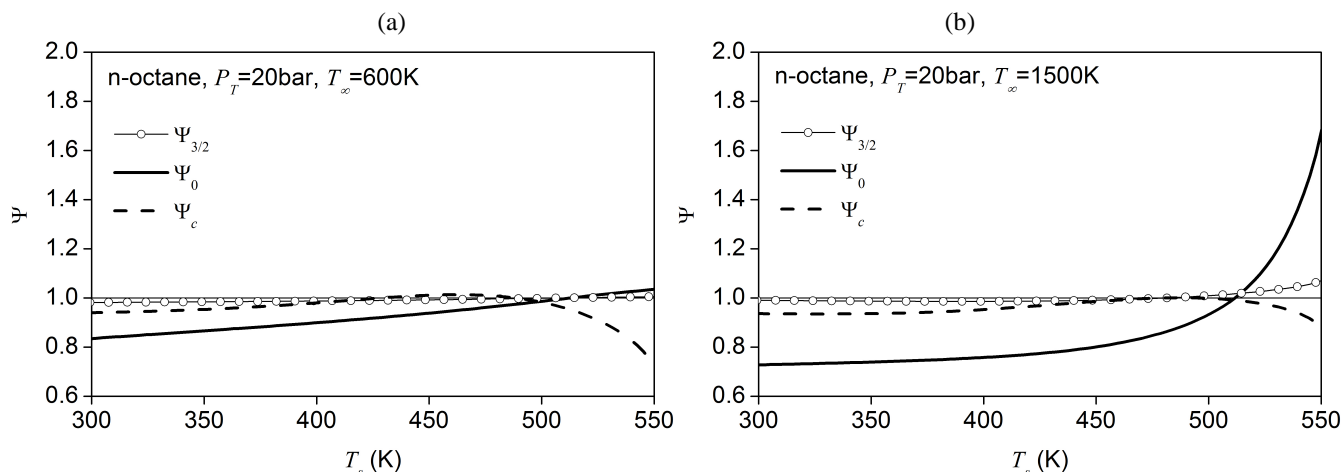
The effect of high gas pressure is reported in figure 4 for the case of n-octane drop vaporising at 20bar and the two gas temperatures selected in figure 3, evidencing that only the variable density model shows a substantial reduction on the evaporation rate at drop temperature close to the boiling point. The models have been applied to predict the evaporation rate for other hydrocarbons and the results confirm the previous outcomes (not shown here).



**Figure 2** (a) Evaporation rate ratio  $\Psi$  predicted by the four models as function of drop temperature for water drop at 1bar and (a) 500K and (b) 1500K.



**Figure 3** (a) Evaporation rate ratio  $\Psi$  predicted by the four models as function of drop temperature for n-octane drop at 1bar and (a) 600K and (b) 1500K.



**Figure 4** (a) Evaporation rate ratio  $\Psi$  predicted by the four models as function of drop temperature for n-octane drop at 20bar and (a) 600K and (b) 1500K.

## CONCLUSIONS

An analytical model has been developed predicting the evaporation rate from a drop under quasi-steady conditions, accounting for the temperature dependence of mixture density and diffusion coefficient. The evaporation rate for water and hydrocarbon drops at different drop and gas temperature and pressure is calculated by the present model and the results are compared with the predictions from the variable density model, previously developed by the Authors, and by the classical constant property model. The results evidence that the selection of the exponent for the power law dependence of the diffusion coefficient on the absolute temperature may have an effect only at evaporating conditions close to the boiling point. Accounting only for the temperature dependence of density on the evaporation rate predictions yields more visibly discrepancy compared to the case of constant property, due to the different dependence of density and diffusion coefficient with temperature. The discrepancies are enlighten under highly evaporating conditions and particularly for hydrocarbon drops.

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