VAPORIZATION OF MULTI-COMPONENT DROPLETS USING CONTINUOUS THERMODYNAMICS MODEL WITH MULTIPLE DISTRIBUTION FUNCTIONS

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ABSTRACT

This paper presents a theoretical study on the vaporization of multi-component isolated droplets in high ambient temperature. The liquid mixture is composed of 25 components divided into 3 groups: 11 alcanes, 7 aromatics and 7 naphtenes. Two different models are used to represent this composition, the first one assumes a discrete mixture and considers each individual species, and the second uses a distribution function for each group of homogenous components.

The aim of this study is to investigate the numerical predictions of the different models and their computation time. The most significant results concern the vapor flow rates since the vapor composition in combustion chambers affects the combustion behavior (ignition, flame propagation, flame stability…). For the major components, both models predict the same results and deviations appear only for minor components. However, the second model requires less computational time and proves to be more applicable in spray calculations with real fuel drops.

INTRODUCTION

The improvement of combustors and engine performances and the reduction of pollutant emissions require a better understanding of the vaporization process inside the spray. Commercial fuels are complex blends composed of hundreds components, but most works on multi-component droplets assume only a few components, which cannot accurately reproduce the evaporation of a complex liquid mixture with components covering a wide range of boiling points.

The first models of vaporizing multi-component droplets [1,2], called "Discrete Components Models" (DCM), consider each individual species. Since the computation time increases considerably with the number of components inside the droplet, these models are not appropriated to simulate the evaporation of a real fuel spray. To overcome this problem, Tamim and Hallett [3] and Hallett [4] proposed the "Continuous Thermodynamics Models" (CTM) to simplify the mixture by describing the composition by a Probability Distribution Function (PDF) of the molecular weight. However, a PDF represents only one group of homogenous components, each having different distribution parameters and physical properties. Hallett and Grimwood [5] and Abdel-Qadar and Hallett [6] improved the CTM to describe the mixture with as many PDF as the number of groups of homogenous components, and the composition profile inside the drop is governed by infinite or limit/effective diffusion models.

In the litterature, DCM and CTM are rarely compared [7,8] and the liquid blend is only represented by one PDF. To fill this lack, the vaporization of an alcane-aromatic-naphtene mixture is studied with both models using infinite diffusion and diffusion limit models.

MODELING

Discrete Components Models

In DCM, each component present in the liquid or vapor phase has its own mole fraction and requires separate transport equation and physical properties and, with a large number of components like commercial fuels, the computational time becomes significant.

The models used for the transport of energy and species in the liquid mixture are the infinite diffusion model and the diffusion limit model. The first model assumes that the droplet temperature and composition remain uniform throughout the droplet lifetime, whereas the second model assumes a spherical profile for the droplet temperature and composition governed by the diffusion equations. Both models are completely described by Sirignano [2].

Continuous Thermodynamics Models

The CTM is an extension of the DCM where the components are replaced by groups of homogenous components. Therefore each group j is represented by a PDF $f_j(I)$ with two distribution parameters (the mean θ_j and the variance σ_j), which are sufficient to accurately reproduce the composition. Here the distribution variable I is the species molecular weight. The vapor and liquid mole fractions of a component i are respectively given by:

$$x_{i,v} = x_{j,v} f_{j,v}(I)\Delta I \ \text{ and } \ x_{i,l} = x_{j,l} f_{j,l}(I)\Delta I \tag{1}$$

where $x_{j,v}$ and $x_{j,l}$ are the overall mole fractions of the group j respectively in the vapor and liquid phases, and ΔI is the constant molecular weight step. The PDF f_j is defined by the Γ-distribution:

$$f_j(I) = \frac{(I-\gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp\left[-\left(\frac{I-\gamma}{\beta}\right)\right] \tag{2}$$

$$\theta_j = \alpha\beta + \gamma; \quad \sigma_j^2 = \alpha\beta^2$$

with the following properties:

$$\int_\gamma^\infty f_j(I)dI = 1; \quad \int_\gamma^\infty f_j(I)IdI = \theta_j; \quad \int_\gamma^\infty f_j(I)I^2 dI = \Psi_j = \theta_j^2 + \sigma_j^2 \tag{3}$$

Equations, detailed in [3-6], are deduced by inserting $x_{i,v}$ and $x_{i,l}$ from equation (1) into the equations of the DCM and integrating over the distribution with I^n ($n = 0, 1, 2$) as a weighting function, as done in equations (3).

INITIAL AND AMBIENT CONDITIONS

A 100 μm droplet is initially compounded by 25 species separated into 3 groups: 11 n-alcanes (C_6H_{14} to $C_{16}H_{34}$), 7 benzenes (C_6H_6 to $C_{12}H_{18}$) and 7 cyclohexanes (C_6H_{12} to $C_{12}H_{24}$). To compare both liquid modelings, the initial values of liquid mole fractions of the DCM are chosen to correctly fit with the PDF of the CTM (Figure 1). The droplet is placed at the initial temperature of 298 K in stagnant air at the atmospheric pressure and at a temperature of 1000 K. There is no motion between the droplet and the ambient air.
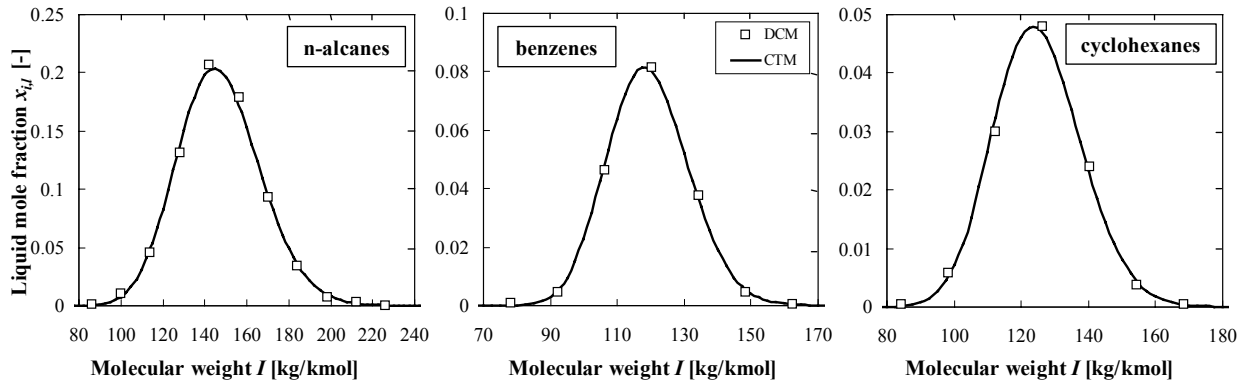

Figure 1: Initial droplet composition

NUMERICAL RESULTS

Figure 2 indicates the temporal evolution of the droplet surface and the surface temperature. It appears that our CTM lightly overestimate the droplet lifetime but underestimate the surface temperature. This can be explained by the assumptions simplifying the CTM. The infinite diffusion and diffusion limit models give close results, except for the surface temperature during the heating phase at the beginning of the vaporization, when the gradients of temperature are not negligible. The uniformity of the liquid temperature for the infinite diffusion models tends to underpredict the droplet surface temperature.
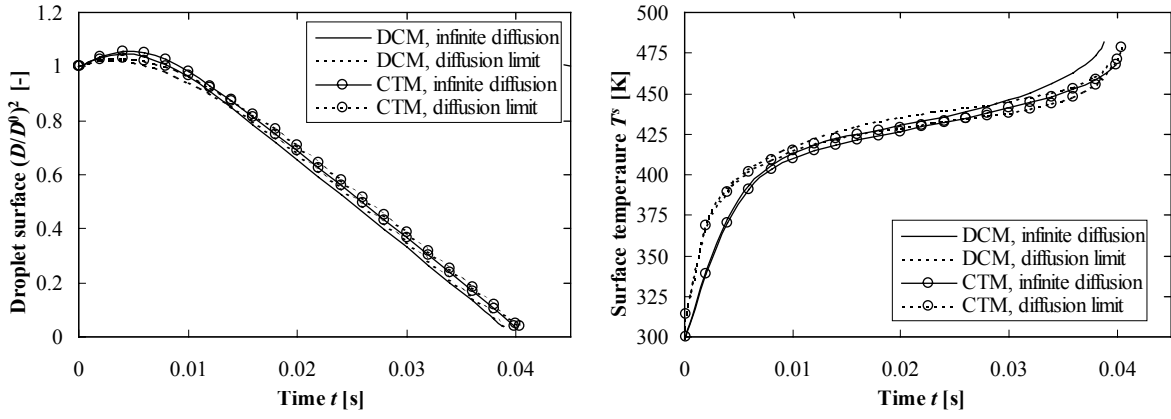
Figure 2: Temporal evolution of the droplet surface (left) and droplet surface temperature (right)

The results of the overall liquid mole fractions at the droplet surface $x_{j,l}^s$ for each group are given in Figure 3. The n-alcanes group covers a range of boiling points (342-560 K) wider than the benzenes and cyclohexanes (respectively 353-499 K and 354-497 K). Therefore the proportions of benzenes and cyclohexanes decrease during the evaporation and the droplet is almost only composed of n-alcanes.
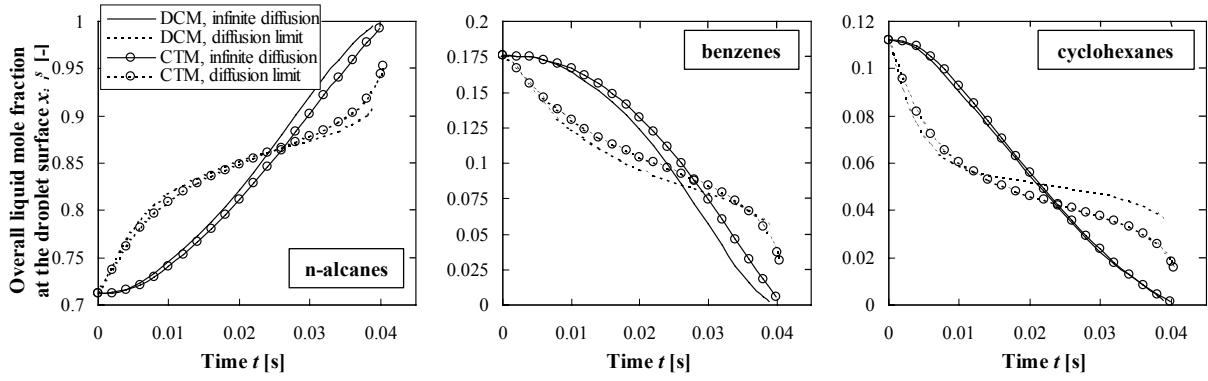

Figure 3: Temporal evolution of the overall liquid mole fraction at the droplet surface

The DCM and the CTM fit correctly, however gaps appear between the infinite diffusion and diffusion limit models. The infinite diffusion model instantaneously transfers liquid species from the center to the surface to make uniform the droplet composition, unlike the diffusion limit model, in which the diffusion limits this transfer. These discrepancies in the composition at the droplet surface have an influence only on the vapor flow rate of benzenes and cyclohexanes (Figure 4), but not on the n-alcanes, since they are the major components and thus, the percentage error on the liquid mole fractions at the surface is lower.
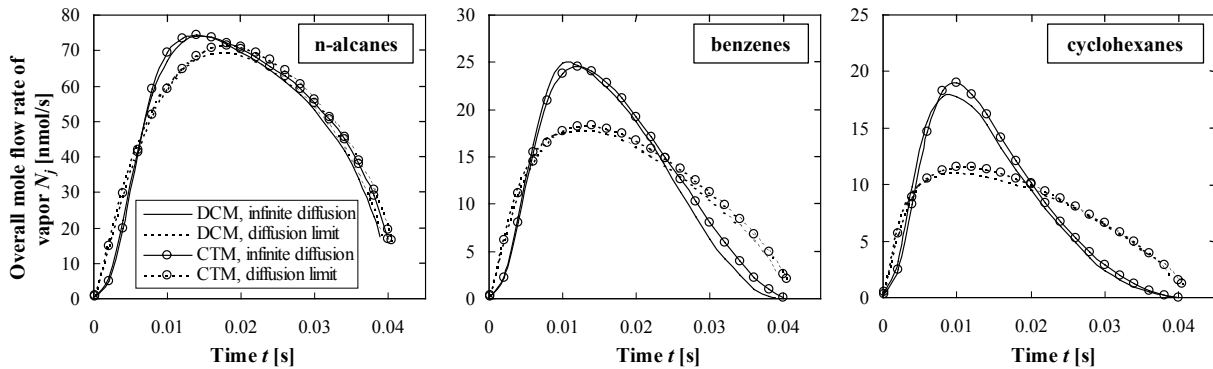

Figure 4: Temporal evolution of the overall mole flow rate of vapor

The distribution parameters of the vapor phase for the DCM are calculated and compared with CTM results in Figure 5. DCM and CTM still fit, except for the variance in the second half of the droplet lifetime for the benzenes and cyclohexanes groups. The mean molecular weight with infinite diffusion model increases in time and the variance is almost constant, that means the components approximately vaporize alternatively. The mean molecular weight slightly increases during a large part of the droplet lifetime with diffusion limit model. We can suppose that the vapor flow rate for minor components slightly varies throughout the droplet lifetime, as opposed to the results of the infinite diffusion model.
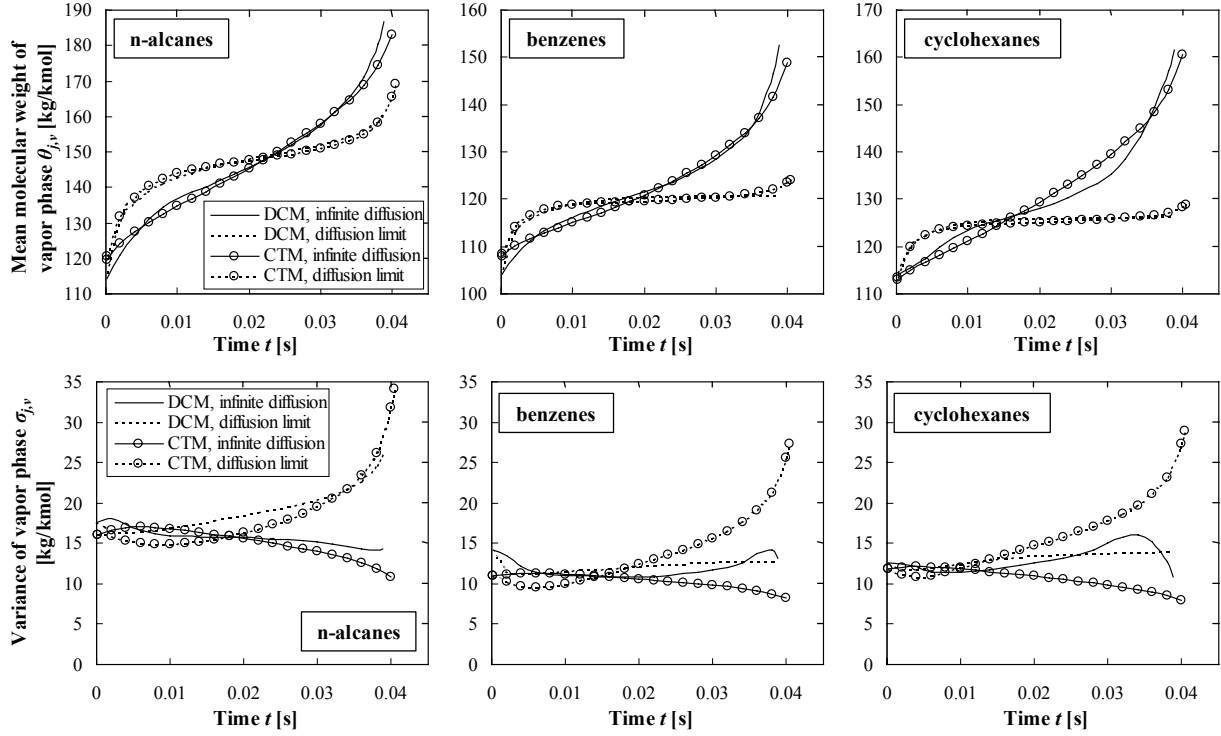

Figure 5: Temporal evolution of the distribution parameters of the vapor phase

For a better comparison of the evaporation phenomena, the PDF of the CTM are discretised using Equation 1. A first observation of these results (Figure 6) shows that the more major is the component in its group, the best the prediction fit. For each group of components, three vaporizing behaviors can be distinguished: the evaporation of the minor components with a low boiling temperature (case 1), the major components (case 2) and the minor components with a high boiling temperature (case 3).

An example of vapor flow rate is given for each case in Figure 6. The components of the first case (example: C_7H_{16} n-alcane in Figure 6) vaporize first. Their liquid mole fractions at the droplet surface initially decrease faster with the diffusion limit model due to the diffusion, which limits the renewal of the vaporized species, unlike the predictions of the infinite diffusion model, in which species are immediately transferred to the droplet surface. However, the previous model completely vaporizes these components before the end of the droplet lifetime (C_7H_{16} n-alcane in Figure 6), whereas the liquid mole fractions with diffusion limit models tend to stabilize, the quantity of liquid diffused to the surface compensating for the quantity vaporized. As these liquid mole fractions were initially low, the difference of liquid species diffusion implies non-negligible discrepancies in liquid and vapor compositions at the droplet surface, that considerably affects the vapor flow rate. The infinite diffusion models entirely vaporize these species for the first half of the droplet lifetime and a peak appears at the beginning of the evaporation, while the diffusion limit model weakly vaporized these components during the whole droplet lifetime (C_7H_{16} n-alcane in Figure 6). The difference between the DCM and the CTM depends on the initial values of the liquid mole fractions, which may considerably vary since the discretisation of the PDF does not give precise initial mole fractions for minor components. The more these initial liquid fractions are close, the more DCM and CTM correctly fit with infinite diffusion models, but diffusion limit model using CTM tends to underestimate the liquid mole fraction and the vapor flow rate (C_7H_{16} n-alcane in Figure 6).

For the major components (case 2), for example the $C_{11}H_{24}$ n-alcane presented in Figure 6, the differences in liquid fractions at the surface between the infinite and diffusion limit models decrease and predict approximately identical behaviors, especially for the n-alcanes vapor flow rate. In fact, the observations done before with the overall vapor flow rates for the groups of components (Figure 4) are the same here. The n-alcanes results best fit, whereas infinite diffusion and diffusion limit predict little differences for other two groups.

For the components of the third case, results for the n-alcanes and the other two groups must be described separately. The n-alcanes of this case vaporize lately since they have the highest boiling temperatures in the mixture. In

the last quarter of the droplet lifetime, there are almost no benzenes and cyclohexanes left, and it becomes difficult to represent the composition of these groups with a PDF. The infinite diffusion models predict identical behaviors for the $C_{11}H_{16}$ benzene (Figure 6) and $C_{11}H_{22}$ cyclohexane, unlike the diffusion limit models, in which CTM converges at the end of the droplet lifetime on the CTM using infinite diffusion model. For the last components ($C_{12}H_{18}$ benzene and $C_{12}H_{24}$ cyclohexane), the CTM cannot reproduce the results of the DCM. Concerning the n-alcanes (for example $C_{14}H_{30}$ n-alcane in Figure 6), the infinite diffusion models values present a peak at the end of the droplet lifetime, whereas the vapor flow rates with the diffusion limit models increase slower. The reason for this difference is the same as the one described for the components of the first case (species transport to the surface). The vapor flow rate predicted by all the models converges for the last components ($C_{15}H_{32}$ n-alcane and $C_{16}H_{34}$ n-alcane), except the CTM using diffusion limit model.
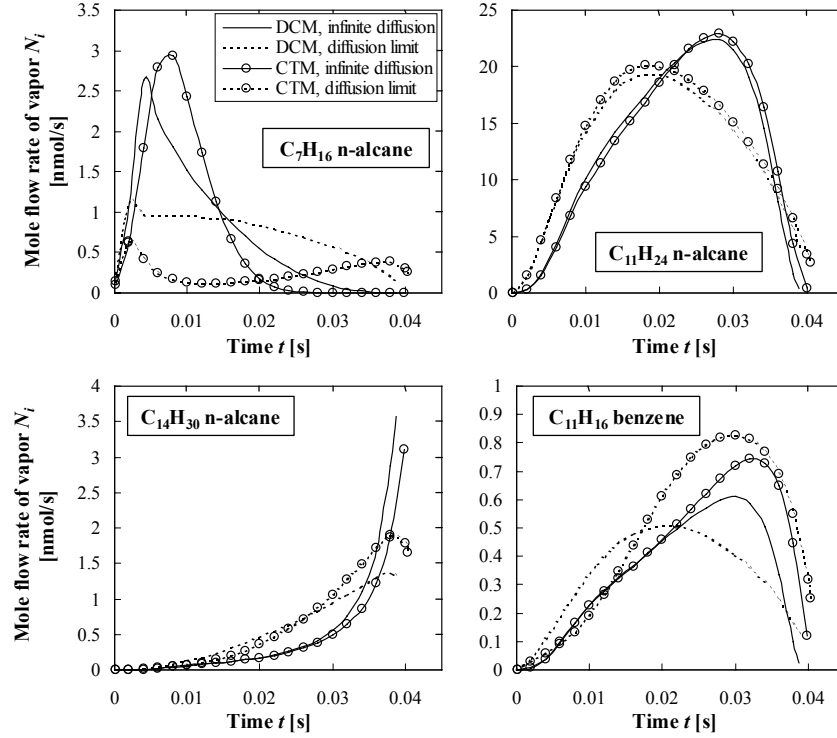

Figure 6: Examples of temporal evolution of vapor mole flow rate for individual species

Table 1 clearly shows the gain of time of the CTM with multiple distribution functions. The computation time is divided by 10 with the infinite diffusion model and by 4 with the diffusion limit model. The time step used is 1 μs, but all the models can run at 100 μs.

Liquid model	Diffusion model	Computation time [s]
DCM	Infinite	57
	Limit	173
CTM	Infinite	6
	Limit	41

Table 1: Computation time for the different models

CONCLUSION

In the present study, different models of the vaporization of a complex liquid mixture with different homogenous groups were compared. With such a number of components, a discrete description of the liquid modeling requires too much computation effort to be included in spray calculations, even with uniform temperature and composition assumptions. The groups of homogenous components, having different chemical properties, cannot be correctly modeled by only one PDF. A continuous approach of the liquid composition with multiple PDF reproduces accurately the vaporizing process predicted by the discrete approach, especially supposing that the temperature and the composition are uniform. This last assumption considerably reduces the computation time and its effects on the vaporization of major components are weak.

An extension of this work is the introduction of these models in spray calculation codes to simulate, for example, the composition of the vapor phase in combustion chambers, just before the ignition and the flame propagation.

NOMENCLATURE

Latin Letters

D	droplet diameter	[m]
$f(I)$	distribution function	[dimensionless]
I	distribution variable, = molecular weight	[kg/kmol]
N	vaporizing mole flow rate	[nmol/s]
x	mole fraction	[dimensionless]

Greek Symbols

α	parameter of the PDF	[dimensionless]
β	parameter of the PDF	[dimensionless]
γ	parameter of the PDF	[dimensionless]
Γ	gamma function	[dimensionless]
ΔI	molecular weight step	[kg/kmol]
θ	mean molecular weight	[kg/kmol]
σ	variance	[kg/kmol]
Ψ	distribution second central moment (= $\theta^2 + \sigma^2$)	[(kg/kmol)^2]

Subscripts and Superscripts

i	individual component
j	group of homogenous components
l	liquid
s	surface
v	vapor
0	initial state

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