

Combustion for aerospace propulsion

Continuous thermodynamics for droplet vaporization: Comparison between Gamma-PDF model and QMoM

Claire Laurent *, Gérard Lavergne, Philippe Villedieu

ONERA/DMAE, 2, avenue Edouard-Belin, BP 74025, 31055 Toulouse cedex 4, France

Available online 21 July 2009

Abstract

The *Continuous Thermodynamics Model* (CTM) (Cotterman et al., 1985) is a suitable method to reduce computational cost of multi-component vaporization models. The droplet composition is described by a probability density function (PDF) rather than tens of components in the classical *Discrete Component Model* (DCM). In the first CTM method developed for this application, the PDF was assumed to be a Γ -function (Hallett, 2000), but some problems had appeared in the case of vapor condensation at the droplet surface (Harstadt et al., 2003). The method put forward in this article, the *Quadrature Method of Moments* (QMoM), enables one to avoid any assumption on the PDF mathematical form. Following Lage who has developed this method for phase equilibria (Lage, 2007), this article widens the scope of QMoM to the modelling of multi-component droplet vaporization. The different CTM approaches are presented in the first part and the results obtained for a vapor condensation test case are then compared and analysed to illustrate improvements made by QMoM. **To cite this article:** C. Laurent et al., *C. R. Mecanique* 337 (2009).

© 2009 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

Résumé

Modélisation de l'évaporation des gouttes en thermodynamique continue : comparaison entre le modèle Gamma-PDF et la QMoM. La modélisation à *Thermodynamique Continue* (MTC) (Cotterman et al., 1985) est une méthode appropriée pour réduire les coûts de calcul associés à la modélisation de l'évaporation multi-composant. La composition des gouttes est modélisée par une fonction de distribution qui représente les dizaines d'espèces prises en compte par le modèle classique à *Composants Discrets* (MCD). Dans la première approche à *Thermodynamique Continue* développée pour cette application, la composition du mélange était décrite par une fonction de distribution de type fonction Γ (Hallett, 2000). Cependant, cette approche a été mise en défaut dès lors que de la vapeur se condensait à la surface de la goutte (Harstadt et al., 2003). La méthode proposée dans cet article, dite de *Quadrature des Moments*, permet d'éviter toute hypothèse sur la forme de la fonction de distribution. A partir des travaux de Lage qui a appliqué cette méthode à l'équilibre thermodynamique des phases (Lage, 2007), ce papier élargit le domaine d'application de la QMoM à l'évaporation des gouttes multi-composant. Les différentes approches à *Thermodynamique Continue* sont décrites dans la première partie et les résultats obtenus dans un cas de condensation de vapeur sont ensuite comparés et analysés pour illustrer les améliorations apportées par la QMoM. **Pour citer cet article :** C. Laurent et al., *C. R. Mecanique* 337 (2009).

© 2009 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

Keywords: Combustion; Multi-component droplet; Vaporization; Continuous thermodynamics; Gamma-PDF model; Quadrature Method of Moments

Mots-clés : Combustion ; Gouttelette multi-composant ; Evaporation ; Thermodynamique continue ; Modèle Gamma-PDF ; Méthode de Quadrature des Moments

* Corresponding author.

E-mail addresses: claire.laurent@onera.fr (C. Laurent), gerard.lavergne@onera.fr (G. Lavergne), philippe.villedieu@onera.fr (P. Villedieu).

1. Introduction

The droplet composition can have a real impact on the vapor flow rate, at low temperature for example with a pronounced distillation effect, or in the case of a mixture composed of components whose physical properties are very different. An example for aero-engine manufacturers is the high-altitude engine relighting, which is a critical issue for the combustion chamber conception. Bio-fuels, which may be complex mixtures of various components, are another application field for the modelling of multi-component droplet vaporization.

Several approaches have been developed to compute fuel composition during the droplet vaporization process. The classical model, called *Discrete Component Model* (DCM), solves evolution equations for each fuel component [1]. However, fuels such as kerosene, diesel or gasoline are composed of tens of compounds and this model is much too time consuming to be implemented in industrial codes. Therefore, some models in which the composition is described by a probability density function (PDF) have been investigated. This approach, called *Continuous Thermodynamic Model* (CTM), is relevant to reduce computational costs. In this way, Hallett developed a model for vaporizing droplets assuming that the PDF is a Γ -function [2], as Cotterman previously did for multi-component vapor–liquid equilibrium [3]. Nevertheless, if vapor condenses on the droplet surface, the PDF shape can be very different from a Γ -function and this model fails [4]. As this phenomenon can occur in combustion chambers, new methods which avoid hypotheses on the PDF mathematical form [5] have been recently studied, like the Orthogonal Collocation (OC) developed by Arias-Zugasti and Rosner [5]. The method proposed here, the *Quadrature Method of Moments* (QMoM), has the same feature and some other remarkable properties too, as, for example, robustness, which is a crucial point for implementation in CFD codes. The QMoM has already been applied by Lage to describe the multi-component vapor–liquid equilibrium [6], and this method is now extended to droplet vaporization modelling, as Hallett has previously done from Cotterman scientific work [2,3]. The QMoM has already been implemented successfully in other fields too, like aerosol dynamics [7] and population balance equations [8].

This article presents first a description of these different approaches and then, a comparison between models for the difficult test case of vapor condensation at the droplet surface.

2. Vaporized droplet composition modelling

2.1. Description of the droplet composition

During the vaporization process, the droplet composition is changing because of the volatility difference between the fuel components. This modification is significant for the vapor flow rate calculation. The objective of the *Continuous Thermodynamic Model* (CTM) is to recover a continuous description of the liquid composition. The PDF f_l is defined by the equation $x_l^i = f_l(I)\Delta I$, where x_l^i represents the mole fraction of the real component i and I the corresponding distribution parameter. The chosen distribution parameter I is the normal boiling point (i.e., $I = T_{nb}$), which is a suitable variable to characterize a component for vaporization process. Indeed, contrary to the molar mass which is commonly used [2,4], the normal boiling point is a direct parameter for saturation vapor pressure and heat of vaporisation (see Eqs. (20) and (21)).

The first studied *Continuous Thermodynamic Model* presumed the mathematical form of the droplet composition PDF as a Γ function. This is the Γ -CTM approach, and the droplet composition PDF is modelled as follows [2,3]:

$$f_l(I) = x_l \frac{(I - \gamma)^{\alpha_l - 1}}{(\beta_l)^{\alpha_l} \Gamma(\alpha_l)} \exp\left(-\left(\frac{I - \gamma}{\beta_l}\right)\right) \quad (1)$$

The second method put forward in this paper is the *Quadrature Method of Moments* (QMoM). The droplet composition PDF is then discrete and the QMoM can be interpreted as a *Discrete Component Model* with N pseudo-components instead of \mathcal{N} real components with $N \ll \mathcal{N}$. The normal boiling point of each pseudo-component may change during the vaporization process [6]. The PDF describing droplet composition in QMoM approach is therefore:

$$f_{l,N}(I) = \sum_{k=1}^N \hat{x}_l^k \delta_{f_l^k}(I) \quad (2)$$

The α order moments of the droplet composition PDF are defined by:

$$m_l^\alpha = \int_0^{+\infty} f_l(I) I^\alpha dI \quad (3)$$

The moments are obtained from the integrated form of the classical equations describing droplet composition evolution during vaporization. Consequently, the physical properties have to be interpolated as functions of $I = T_{nb}$. In case of complex mixtures, the components are classified into homogeneous groups as alkanes, alcohols or monoaromatics in order to ensure a satisfying modelling of each group's physical behaviour. This is the first hypothesis of the *Continuous Thermodynamic Models* (**Hypothesis 1**). The pseudo-components have therefore variable physical properties depending on their boiling point. This method allows one to use 2 or 3 pseudo-components for each homogeneous group instead of tens real components for the whole mixture. In the following section, the models are only detailed for one group of components, since the multiple PDF model is merely an extension which uses classical DCM approach applied to groups instead of components.

2.2. Droplet composition evolution

In the DCM approach, the evolution of the fuel composition in the droplet during the vaporization process is described by

$$\frac{dx_l^i}{dt} = \frac{3}{4\pi R^3 c_l} (\dot{n}_{tot} x_l^i - \dot{n}^i) \quad (4)$$

These equations are written using the molar system since it is more convenient for *Continuous Thermodynamic* methods. Then, c_l represents the molar density of the droplet and R its radius. The vapor flow rate of each component i is \dot{n}^i and it is the sum of a convection and a diffusion term:

$$\dot{n}^i = \dot{n}_{tot} x_{g,s}^i - 2\pi R c_g D_g^i Sh_g^i (x_{g,\infty}^i - x_{g,s}^i) \quad (5)$$

In this equation, Sh_g^i is the *Sherwood* number which refers to the classical definition,

$$Sh_g^i = \frac{2R}{x_{g,\infty}^i - x_{g,s}^i} \left(\frac{\partial x_g^i}{\partial r} \right)_s \quad (6)$$

and D_g^i is the diffusion coefficient of the component i . The integration performed by the CTM approach leads one to assume that the diffusion coefficient D_g^i and the *Sherwood* number Sh_g^i do not depend on the component (this is the **Hypothesis 2** of the *Continuous Thermodynamic Model*). The continuous form of Eq. (4) using Eq. (5) is then:

$$\frac{df_l(I)}{dt} = \frac{3}{4\pi R^3 c_l} (\dot{n}_{tot} f_l(I) - \dot{n}_{tot} f_{g,s}(I) + 2\pi R c_g D_g Sh_g (f_{g,\infty}(I) - f_{g,s}(I))) \quad (7)$$

The *Spalding* number is commonly used for vaporization models. Its definition is:

$$B_M = \frac{x_{tot}^{g,s} - x_{tot}^{g,\infty}}{1 - x_{tot}^{g,s}} \quad (8)$$

The vapor mole fraction at the droplet surface $x_{tot}^{g,s}$ is obtained from the phase equilibrium at the droplet interface. This point is detailed below in Section 2.4. Then, using the B_M definition and by summing Eq. (5) for all components i , we deduce

$$\dot{n}_{tot} = 2\pi R c_g D_g Sh_g B_M \quad (9)$$

which is equivalent to the well-known equation

$$\dot{n}_{tot} = 2\pi R c_g D_g Sh_g^* \ln(1 + B_M) \quad (10)$$

where Sh_g^* is the *modified Sherwood* number defined by:

$$Sh_g^* = \frac{B_M}{\ln(1 + B_M)} Sh_g \quad (11)$$

For an immobile droplet, $Sh_g^* = 2$ and, in the general case, Sh_g^* is given by correlations depending especially on the *Reynolds* number (see [1]).

All the terms of Eq. (7) have been clarified in order to allow CTM integration and then, the moment equations can be obtained.

2.3. The Moment Problem

The evolution equations for the α order moments m_l^α are carried out by integrating Eq. (7):

$$\frac{dm_l^\alpha}{dt} = \frac{3}{4\pi R^3 c_l} (\dot{n}_{tot} m_l^\alpha - \dot{n}_{tot} m_{g,s}^\alpha + 2\pi R c_g D_g Sh_g (m_{g,\infty}^\alpha - m_{g,s}^\alpha)) \quad (12)$$

Using Eq. (9), the system can be rewritten as follow for $\dot{n}_{tot} \neq 0$ (i.e., $B_M \neq 0$):

$$\frac{dm_l^\alpha}{dt} = \frac{3\dot{n}_{tot}}{4\pi R^3 c_l} \left(m_l^\alpha - \frac{m_{g,s}^\alpha (1 + B_M) - m_{g,\infty}^\alpha}{B_M} \right) \quad (13)$$

or, for $\dot{n}_{tot} = 0$:

$$\frac{dm_l^\alpha}{dt} = \frac{3c_g D_g Sh_g}{2R^2 c_l} (m_{g,\infty}^\alpha - m_{g,s}^\alpha) \quad (14)$$

The so-called *Moment Problem* consists of computing the droplet composition PDF from a set of moments obtained at each time step from Eq. (13) or Eq. (14).

For the Γ -CTM approach, the PDF is defined by the parameters α_l and β_l (see Eq. (1)) which can be calculated from the mean normal boiling point Θ_l and the standard deviation σ_l or from the first and the second order moments m_l^1 and m_l^2 :

$$\left\{ \begin{array}{l} \alpha_l = \left(\frac{\Theta_l - \gamma}{\sigma_l} \right)^2 = \frac{(m_l^1 - \gamma)^2}{m_l^2 - (m_l^1)^2} \\ \beta_l = \frac{(\sigma_l)^2}{(\Theta_l - \gamma)} = \frac{m_l^2 - (m_l^1)^2}{m_l^1 - \gamma} \end{array} \right. \quad (15a)$$

$$\quad (15b)$$

When the *Quadrature Method of Moments* is used, the solution is obtained by computing the nodes $\{\hat{I}_l^k\}_1^N$ and the weights $\{\hat{x}_l^k\}_1^N$ of a *Gauss quadrature* whose formulation for its application to $f_{l,N}$ is

$$\int F(I) f_{l,N}(I) dI = \sum_{k=1}^N \hat{x}_l^k F(\hat{I}_l^k) + \mathcal{R}(F) \quad (16)$$

$$\mathcal{R}(\mathbb{P}^{2N-1}) = 0 \quad (17)$$

Indeed, the moment problem studied corresponds to $F(I) = I^\alpha$ and consequently, the *Gauss Quadrature* gives an exact solution for moments up to the $2N - 1$ order. This *quadrature rule* is optimal, N nodes are necessary and sufficient to obtain the $2N$ first moments and the number of nodes required is minimum.

2.4. Vapor–liquid equilibrium at the droplet surface

The model closure is given by the vapor–liquid equilibrium. For ideal mixtures, the phase equilibrium at the droplet surface finds expression in the well-known *Raoult's law*,

$$x_{g,s}^i P_\infty = x_l^i P_{sat}^i(T_s) \quad (18)$$

where $P_{sat}(T_s)$ refers to the saturation vapor pressure expressed at T_s , the temperature at the droplet surface. The continuous form of Eq. (18) is

$$f_{g,s}(I) P_\infty = f_l(I) P_{sat}(I, T_s) \quad (19)$$

and P_{sat} is given, for instance, by the *Clausius–Clapeyron* equation:

$$P_{sat}(I, T_s) = P_\infty \exp\left(\frac{l_{vb}(I)}{\mathcal{R}} \left(\frac{1}{I} - \frac{1}{T_s}\right)\right) \tag{20}$$

The function $(I \rightarrow l_{vb}(I))$ has been interpolated from the normal molar latent heats of vaporization l_{vb} of real components. This enables one to compute the molar latent heat of vaporization, whose classical expression in the literature is [9]:

$$l_v(I) = l_{vb}(I) \left(\frac{T_c(I) - T_s}{T_c(I) - I}\right)^{0.38} \tag{21}$$

where T_c is the critical temperature expressed as a function of I .

The non-polynomial function for $(I \rightarrow P_{sat}(I))$ reveals that integration of the vapor–liquid equilibrium equation is a difficult point, depending on the chosen method (see Eq. (19)). Therefore, the relationship between the moments of the droplet composition and those of the vapor composition does not appear explicitly. For the Γ -CTM approach, this was solved by Cotterman [3] and then resumed by Hallett for the vaporizing droplet modelling [2]. Concerning the method proposed in this paper, the mole fraction \hat{x}_l^k and the normal boiling point \hat{I}_l^k of each pseudo-component are computed with QMoM. Then, using the definition of $f_{l,N}$ (see Eq. (2)), the integration of the continuous form of the *Raoult’s law* (see Eq. (19)) gives the moments of the vapor composition PDF at the droplet surface:

$$m_{g,s}^\alpha = \sum_{k=1}^N \hat{x}_l^k \frac{P_{sat}(\hat{I}_l^k, T_s)}{P_\infty} (\hat{I}_l^k)^\alpha \tag{22}$$

Now, the next step for the *Quadrature Method of Moments* is the computations of nodes $\{\hat{I}_l^k\}_1^N$ and weights $\{\hat{x}_l^k\}_1^N$ from the moments $\{m_l^\alpha\}_0^{2N-1}$.

2.5. Computation of the QMoM nodes and weights

The nodes are solution of the *Gauss quadrature rule* (see Eq. (16)). According to the fundamental theorem of Gauss quadrature [11,12], the nodes $\{\hat{I}_l^k\}_1^N$ are then the roots of the monic orthogonal polynomial π_N relative to the inner product defined by:

$$\langle p, q \rangle = \int_0^{+\infty} p(I)q(I) f_{l,N}(I) dI \tag{23}$$

Now, as any orthogonal sequence has a recurrence formula relating any three consecutive terms, the following relation appears for the $\{\pi_k\}_{-1}^N$:

$$\begin{cases} \pi_{k+1} = (I - a_k)\pi_k - b_k\pi_{k-1} \end{cases} \tag{24a}$$

$$\begin{cases} \pi_{-1} = 0 \end{cases} \tag{24b}$$

$$\begin{cases} \pi_0 = 1 \end{cases} \tag{24c}$$

The key point of the QMoM algorithm is then to compute the coefficients $\{a_k\}_0^{N-1}$ and $\{b_k\}_1^{N-1}$ from the moments $\{m_l^\alpha\}_0^{2N-1}$ with an efficient method. The *Product-Difference algorithm* developed by Gordon is an effective way to obtain these coefficients [7,10]. Then, the last step is to solve the roots of the monic orthogonal polynomial π_N from a_k and b_k coefficients. Some numerical methods are described in literature. Indeed, the roots of the polynomial π_N are the eigenvalues of a tridiagonal matrix built from a_k and b_k coefficients [11,12]. In this way, the normal boiling points $\{\hat{I}_l^k\}_1^N$ are computed from the $2N$ first moments. The mole fractions $\{\hat{x}_l^k\}_1^N$ are then easily deduced.

3. Results analysis

3.1. Test case description

In this study, the *Discrete Component Model* (DCM), which solves droplet composition for each real component of the mixture, is considered as the reference model. The test case presented below has been chosen for its difficulty. Its

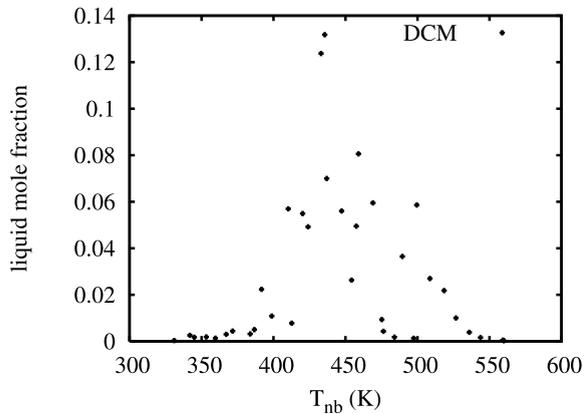


Fig. 1. Kerosene PDF for the *Discrete Component Model* (36 components).

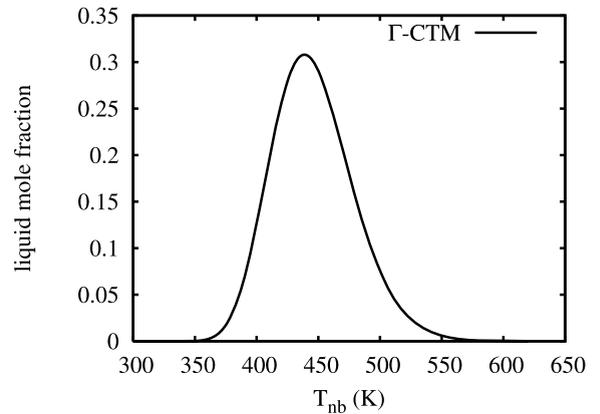


Fig. 2. Kerosene PDF for the Γ -*Continuous Thermodynamic Model*.

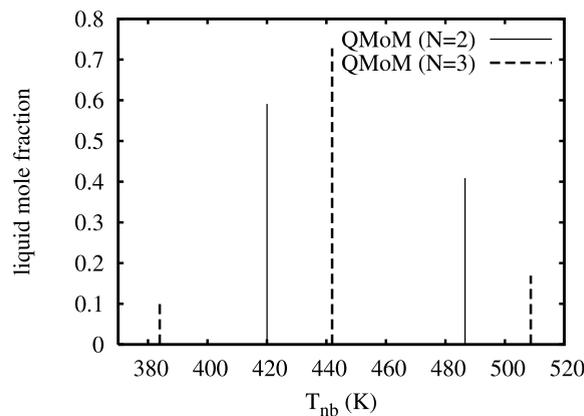


Fig. 3. Kerosene PDFs for the *Quadrature Method of Moments* ($N = 2$ and $N = 3$).

objective is to assess the QMoM when vapor condenses at the droplet surface, and consequently to prove its robustness in this case contrary to Γ -CTM approach [4].

The example application considered in this paper is a kerosene droplet vaporizing in air rich in iso-C₆H₁₄. Indeed, this isoHexane is one of the most volatile component present in kerosene ($T_{nb} = 331$ K). The droplet is 50 μm diameter and its initial temperature is 300 K. The surrounding gas temperature is 500 K and the ambient pressure is 5 bar. The composition of the carrier gas is supposed to be constant: $x_{g,\infty}^{air} = 0.7$ and $x_{g,\infty}^{iso-C_6H_{14}} = 0.3$. Consequently, the PDF $f_{g,\infty}$ of the vapor in the gas phase is reduced to one δ -function. Finally, concerning the liquid phase, the initial PDFs of the droplet composition are plotted on Fig. 1 for the *Discrete Component Model* (DCM), on Fig. 2 for the Γ -*Continuous Thermodynamic Model* (Γ -CTM) and on Fig. 3 for the *Quadrature Method of Moments* (QMoM).

3.2. Comparison between the different approaches

Computations using the different models have been performed and the results are now analysed. The first physical parameter studied is the vapor flow rate (see evolution on Fig. 4). The vapor (iso-C₆H₁₄) first condenses (i.e., the vapor flow rate is negative) and then, when the droplet is rich enough in iso-C₆H₁₄, it evaporates (i.e., the vapor flow rate is positive). In comparison to the Γ -CTM approach, the QMoM results are closer to the reference model (DCM) than Γ -CTM and, as expected, this is improved by increasing the number of pseudo-components (i.e., $N = 3$ instead of $N = 2$). The droplet temperature evolution is another relevant parameter to study the reliability of models for the thermal aspect (see Fig. 5). The displayed results underline that a failure of the droplet composition model can imply significant errors for other variables too, such as the droplet temperature, for example.

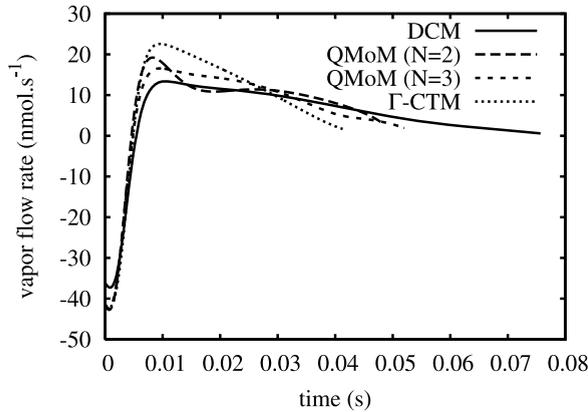


Fig. 4. Comparison between models for the droplet vapor flow rate.

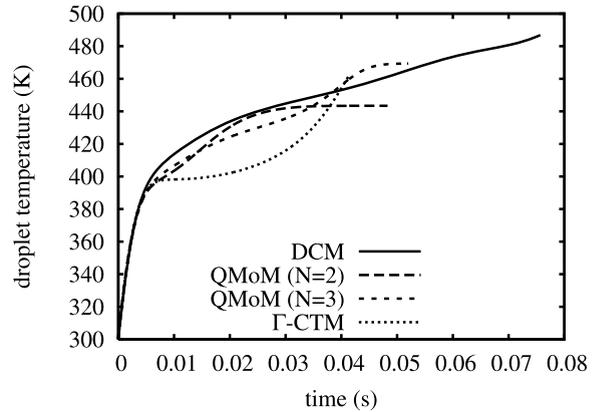


Fig. 5. Comparison between models for the droplet temperature.

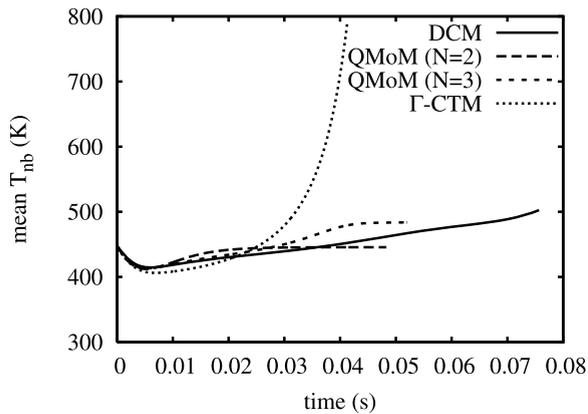
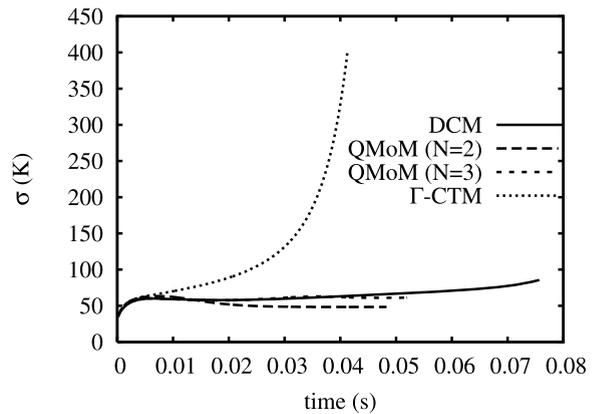
Fig. 6. Comparison between models for the first order moment (mean T_{nb}).

Fig. 7. Comparison between models for the standard deviation.

The failure of the Γ -CTM approach can be studied from the moments evolution. The droplet mean normal boiling point (i.e., the first order moment m_1^l) is thus plotted on Fig. 6. A large discrepancy appears with the Γ -CTM approach, mainly due to the hypothesis on the PDF shape (i.e., the Γ -function assumption). Indeed, after the condensation of the iso- C_6H_{14} on the droplet, the liquid composition PDF has two maxima, one corresponding to the iso- C_6H_{14} concentration and the other to the kerosene composition (see Fig. 8). Consequently, this configuration cannot be represented correctly by a single Γ -function whose standard deviation is consequently too high (see Fig. 7). The droplet composition (i.e., its moments) is therefore much more accurately described using the QMoM instead of the Γ -CTM.

Concerning CPU time, the QMoM is slightly less efficient than the Γ -CTM (see Table 1), due to the algorithm used for finding eigenvalues of a tridiagonal matrix in the QMoM algorithm. Nevertheless, the *Moment Problem* can be analytically solved for 2 pseudo-components ($N = 2$) and the QMoM has then the same computation time as the Γ -CTM. Consequently, the QMoM ($N = 2$) can be a compromise solution for implementation in industrial codes if the computation time turns out to be a very strong constraint.

3.3. Analysis of CTM hypotheses

It is worth noticing that the *Continuous Thermodynamic Model* (both Γ -CTM and QMoM approaches) underestimates the droplet lifetime. Indeed, the CTM rests on two main hypotheses, the first concerns the interpolation of physical properties (**Hypothesis 1**) and the second assumes an identical *Sherwood* number and diffusion coefficient for each component of the same group (**Hypothesis 2**). This last approximation is equivalent to assuming the same

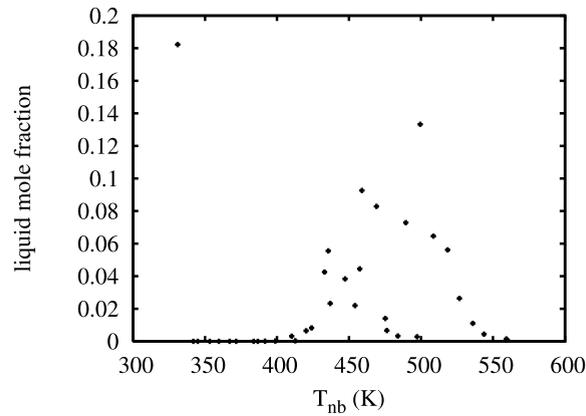


Fig. 8. Kerosene PDF for the *Discrete Component Model* at $t = 0.04$ s.

Table 1

Computation times of the different models.

Model	CPU time
DCM (36 components)	14.6
Γ -CTM	0.6
QMoM ($N = 2$)	0.9
QMoM ($N = 3$)	1.1

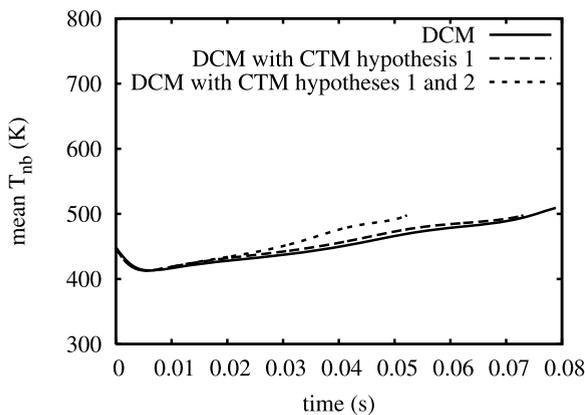


Fig. 9. CTM error analysis for the first order moment (mean T_{nb}).

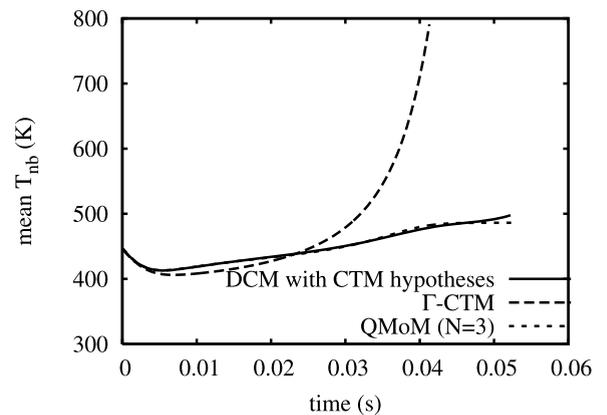


Fig. 10. Comparison between methods to solve CTM approach considering best conceivable solution obtained for the first order moment (mean T_{nb}).

Spalding numbers for all components in the same component group (see Eq. (9)). The results plotted on Fig. 9 underline that the **Hypothesis 2** is the more significant source of error. Indeed, the vapor flow rate is mainly composed of iso-C₆H₁₄. The *Spalding* number value computed with CTM approach is characteristic of a volatile component and this implies an early vaporization of “heavy” components, and consequently a shortening of droplet lifetime. Finally, the performance of QMoM can be estimated from the comparisons with the DCM results computed with CTM hypotheses (see Fig. 10). This underlines that QMoM modelling with 3 pseudo-components ($N = 3$) is very close from the best solution which can be obtained with a CTM approach.

4. Concluding remarks

This article puts forward a new method to solve the *Continuous Thermodynamic* approach of multi-component droplet vaporization modelling. This method, the *Quadrature Method of Moment* (QMoM), has already been applied

by Lage to describe the phase equilibria in order to avoid any assumption on the mathematical form of the droplet composition PDF [6]. The implementation of QMoM is now extended to droplet vaporization modelling, particularly to solve the difficult test case of vapor condensation. Indeed, even though this phenomenon is not preponderant for combustion applications, this case is relevant for numerical purposes. Partial condensation may occur in combustion chambers due to inhomogeneities in the temperature or component mass fraction fields, and then leads to the failure of computations if a classical Γ -CTM approach is used. The robustness required by CFD codes implies finding a method which succeeds in this case. The results obtained with the QMoM have been compared to those given by the Γ -CTM approach and they show a net improvement with QMoM. The QMoM solution with 3 pseudo-components is very close to the DCM results computed with CTM hypotheses. This means that QMoM ($N = 3$) gives practically the best conceivable solution provided by a CTM approach. The computational cost of QMoM ($N = 3$) is furthermore low enough to consider this method to be an acceptable compromise for CFD implementation. The QMoM is consequently very promising for solving the droplet composition modelling issue in industrial codes.

Acknowledgements

The authors are grateful to the ASTRA program founded by CNRS and ONERA. This program concerns the study of multi-component sprays.

References

- [1] W.A. Sirignano, Fluid Dynamics and Transport of Droplets and Sprays, Cambridge University Press, 1999.
- [2] W.L.H. Hallett, A simple model for the vaporization of droplets with large numbers of components, *Combust. Flame* 121 (2000) 334–344.
- [3] R.L. Cotterman, R. Bender, J.M. Prausnitz, Phase equilibria for mixtures containing very many components. Development and applications of continuous thermodynamics for chemical process design, *Ind. Eng. Chem. Process Des. Dev.* 24 (1985) 194–203.
- [4] K.G. Harstadt, P. Le Clercq, J. Bellan, Statistical model of multicomponent-fuel drop evaporation for many-droplet liquid-gas flow simulations, *AIAA J.* 41 (2003) 1858–1874.
- [5] M. Arias-Zugasti, D.E. Rosner, Multi-component fuel droplet vaporization and combustion using spectral continuous mixture theory, *Combust. Flame* 135 (2003) 271–284.
- [6] P.L.C. Lage, The quadrature method of moments for continuous thermodynamics, *Comput. Chem. Eng.* 31 (2007) 782–799.
- [7] R. McGraw, Description of aerosol dynamics by the quadrature method of moments, *Aerosol Sci. Technol.* 27 (1997) 255–265.
- [8] D.L. Marchisio, R.O. Fox, Solution of population balance equations using the direct quadrature method of moments, *J. Aerosol Sci.* 36 (2005) 43–73.
- [9] R.C. Reid, J.M. Prausnitz, T.K. Sherwood, *The Properties of Gases and Liquids*, 3rd edition, McGraw–Hill Book Company, 2009.
- [10] R.G. Gordon, Error bounds in equilibrium statistical mechanics, *J. Math. Phys.* 9 (1968) 655–663.
- [11] W. Gautschi, *Orthogonal Polynomial — Computation and Approximation*, Oxford University Press, 2004.
- [12] W.H. Press, S.A. Teukolsky, Orthogonal polynomials and Gaussian quadrature with nonclassical weight, *Comput. Phys.* 4 (1990) 423–426.