Int. J. Heat Mass Transfer. Vol. 34, No. 11, pp. 2805–2812, 1991
Printed in Great Britain

0017–9310/91 $3.00+0.00
Pergamon Press plc

On the Lagrangian simulation of turbulence influence on droplet evaporation

ALAIN BERLEMONT, MARIE-SOPHIE GRANCHER and GÉRARD GOUESBET
L.E.S.P. UA CNRS 230 INSA de ROUEN, BP 8, 76131 Mt St Aignan Cedex, France

(*Received* 4 *January* 1991 *and in final form* 11 *January* 1991)

Abstract—A Lagrangian approach is developed to study the influence of turbulence on droplet evaporation. Two models can be used for the droplet heating, infinite conductivity and conduction limit. Convection is taken into account by correlation laws, where fluctuating quantities for velocities, temperature or concentration are introduced. The influence of turbulence on the droplet evaporation in homogeneous turbulence is discussed, the results also being compared with simulations which involve mean quantities only.

INTRODUCTION

THE PRESENT paper is concerned with new developments of the code PALAS for the Lagrangian simulation of particle behaviour in turbulent flows. Extensive discussions and validations of the code can be found in refs. [1, 2]. The purpose of this paper is to extend the code to the case of mass transfer between fluid and particles, more precisely to study the influence of turbulence on droplet evaporation.

Research on droplet evaporation is of great importance both on the fundamental and applied points of view. The transfer mechanisms between the liquid phase and the gas phase are quite complex and require specific studies, particularly when the carrier fluid is turbulent.

Evaporation of a single isolated droplet in stagnant surrounding gas has been extensively studied, as reviewed by Faeth [3] and Sirignano [4]. Different models have been developed, from the very simple 'd^2 law' to more realistic approaches such as 'infinite conductivity' or 'conduction limit' models. The problem of droplet evaporation in a convective gas field is more complicated, but has been extensively discussed in the last few years (Prakash and Sirignano [5], Tong and Sirignano [6], Renksizbulut and Haywood [7], and Aggarwal *et al.* [8] among others). These models include more or less sophisticated simulations of the convective processes, but very little work can be found on the influence of the fluid turbulence on droplet evaporation [9].

The aim of this paper is to introduce the instantaneous characteristics of the flow which are encountered by the droplets into the evaporation process. That means the mean quantities of the turbulence are used in the chosen evaporation model, but fluctuating parts of velocities, temperatures or concentrations are considered, using a Lagrangian approach.

The Lagrangian approach is recalled, and the two droplet evaporation models are then described, including the correlation law to account for convection. In the last part of the paper, the influence of the turbulence itself is pointed out by comparing the results with simulations which involve mean quantities only.

Clearly, once the method and corresponding codes are designed, a host of numerical results may be readily obtained and presented. However, to avoid an undue proliferation of figures, we shall select illustrative examples of computations.

THE LAGRANGIAN APPROACH

Although it has been published elsewhere [1, 10], our Lagrangian technique is now briefly presented for completeness.

Fluid particle trajectory

Particle trajectory simulations are different whether fluid or discrete particles are followed. For a fluid particle, its instantaneous velocity can be determined knowing a mean velocity, and by use of random values for the fluctuating part of the velocity. The mean velocity is obtained with a $(k$–$\varepsilon)$ model, but the problem is to determine fluctuating velocities which satisfy the turbulence characteristics.

Assuming a Gaussian pdf for the velocities, a random process is defined, which is 'controlled' through a correlation matrix. The correlation matrix is attached to each fluid particle and memorizes the Lagrangian time correlations along the whole particle trajectory. In our simulations, we are using Frenkiel functions to express the Lagrangian time correlations. These relations depend on the local Lagrangian integral time scale and on a loop parameter which determines the existence and importance of negative loops in the correlation. It is important to mention that the method can be applied whatever the expression which simulates the correlation [11].

Discrete particle trajectory

For a discrete particle, forces acting on the particle are expressed through the Riley [12] equation of motion, which is corrected by classical relations from Odar and Hamilton [13] and Clift *et al.* [14] to take into account non-small particle Reynolds numbers and acceleration numbers.

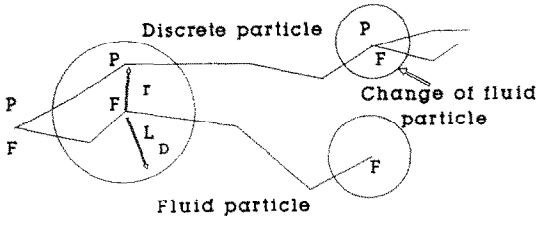
NOMENCLATURE

a	liquid thermal diffusivity
B_M	Spalding mass transfer number
B_T	Spalding heat transfer number
C_D	drag coefficient
C_l	liquid specific heat
C_{vap}	vapour specific heat
D	droplet diameter
D_0	initial droplet diameter
$\mathscr{D}_1$	vapour diffusion coefficient
$\mathbf{g}$	gravity vector
L	latent heat of vaporization
Le_1	vapour Lewis number
M_1	vapour molecular weight
$\dot{m}$	effective mass flow rate
Nu	vaporization Nusselt number
Nu^*	corrected Nusselt number
Pr	Prandtl number
P_{vap}	vapour partial pressure
q_g	heat flow rate on droplet surface
r_s	droplet radius
$\mathscr{R}$	universal gas constant
Re	Reynolds number
Sh^*	corrected Sherwood number
t	time
T, T'	surrounding gas temperature
T_B	boiling point temperature
T^s	droplet surface temperature
T'	r.m.s. temperature
u'	r.m.s. velocity
$\mathbf{U}$	fluid velocity
$\mathbf{V}_p$	droplet velocity
Y, Y_1'	surrounding vapour mass fractions
Y_1^s	droplet surface vapour mass fraction
Y'	r.m.s. vapour concentration.

Greek symbols

Λ	non-dimensional vapour mass flow rate
λ	gas thermal conductivity
ν_{ref}	reference state ('1/3' rule) viscosity
ρ, ρ_f	gas density
ρ_l	liquid density
σ_D	r.m.s. diameter
τ_c	fluid/particle interaction time
τ_L	Lagrangian integral time scale
τ_p	droplet relaxation time.

The main problem to integrate the equation of motion is to determine the instantaneous fluid velocity at the discrete particle location. The process is similar to the method described by Ormancey and Martinon [15]. We follow simultaneously a fluid particle (F) and a discrete particle (P) and Eulerian correlations are used to 'transfer' the turbulence properties from point F to point P.



In that process, we have to take into account the well-known phenomenon of crossing trajectory effects, that is to say the distance between the points F and P must be significant of a correlation domain defined around the fluid particle. We thus define a length scale L_D, taken as a mean value between the transverse and longitudinal Eulerian length scales. When the discrete particle is out of that domain, i.e. when the distance r is larger than L_D, we 'change' the fluid particle. A new fluid particle is considered, starting from the discrete particle location, and the process is then repeated.

The code has been compared with various theoretical and experimental results and has been found to be very satisfactory.

To handle more difficult problems where the influence of the particle on the turbulence is not negligible (high mass loading ratios), a two-way coupling between both phases is effected through momentum and energy exchanges, leading to source terms in the turbulence model ($(k$–$\varepsilon)$ supplemented with algebraic relations for the Reynolds tensor) and to an iterating process. Simulations have been carried out for three different particle laden jets and compared favourably with experiments [1, 2].

DROPLET EVAPORATION MODELS

Assumptions and simplifications

Vaporization phenomena are described in the present study by using 'corrected spherical symmetry', that means spherical symmetry is assumed for heat and mass transfers between the droplet and the surrounding fluid, and convection effects are taken into account by introducing correlation laws in the models.

The main assumptions of the models are [16, 17]:

(a) spherical symmetry;
(b) quasi-steady gas film around the droplet;
(c) uniform physical properties of the surrounding fluid;
(d) uniform pressure around the droplet;
(e) liquid/vapour thermal equilibrium on the droplet surface.

The vapour partial pressure P_{vap} is thus written as

$$P_{vap} = \exp\left[\frac{LM_l}{\mathscr{R}T_B}\left(1-\frac{T_B}{T^s}\right)\right] \quad (1)$$

where L is the latent heat of vaporization, T_B the boiling point temperature of the liquid phase, T^s the droplet surface temperature, M_l the vapour molecular weight and $\mathscr{R}$ the universal gas constant.

The non-dimensional vapour mass flow rate is

$$\Lambda = \frac{2}{Le_l}\ln(1+B_M) \quad \text{with} \quad \Lambda = \frac{\mathring{m}c_{vap}}{\pi D\lambda} \quad (2)$$

where Le_l is the vapour Lewis number

$$Le_l = \frac{\lambda}{C_{vap}\rho\mathscr{D}_l}$$

B_M the Spalding mass transfer number

$$B_M = \frac{Y_l^s - Y_l^\infty}{1-Y_l^s}$$

$\mathring{m}$ the vapour mass flow rate, C_{vap} the specific heat of the vapour, D the droplet diameter, λ the thermal conductivity of the fluid, $\mathscr{D}_l$ the diffusion coefficient of the vapour, and ρ the fluid density. Y_l^s and Y_l^∞ are the vapour mass fraction on the droplet surface and far from the droplet, respectively.

The equation for the droplet diameter is then

$$\frac{dD}{dt} = \frac{-2\Lambda\lambda}{\rho_l D C_{vap}} \quad (3)$$

where ρ_l is the liquid density. To describe the droplet temperature variations, two different models have been used, namely the 'infinite conductivity' and 'conduction limit', as defined by Sirignano [4].

Infinite conductivity model

Assuming that the droplet temperature is uniform, the equation for the droplet temperature variation is

$$\frac{dT^s}{dt} = \frac{6}{D^2}\frac{\lambda}{\rho_l C_l}\times\left[(T^\infty - T^s)Nu - \frac{L}{C_{vap}}\Lambda\right] \quad (4)$$

where C_l is the specific heat of the liquid, T^∞ the fluid temperature, and Nu the Nusselt number defined by

$$Nu = \frac{\dfrac{q_g}{\lambda(T^\infty - T^s)}}{D} = \frac{\Lambda}{\exp(\Lambda/2)-1} \quad (5)$$

where q_g is the heat flow rate on the droplet surface.

Conduction limit model

In the conduction limit model, the droplet temperature is no longer considered to be uniform, but instead the conduction equation is solved inside the droplet.

That equation in a spherical frame of reference is given as follows:

$$\frac{\partial T}{\partial t} = \frac{a}{r_s^2}\left[\frac{\partial^2 T}{\partial x^2}\right] + \frac{1}{r_s^2}\frac{\partial T}{\partial x}\times\left(\frac{2a}{x}+\frac{x}{2}\frac{dr_s^2}{dt}\right) \quad (6)$$

where r_s is the droplet radius, $x = r_0/r_s$ and a is the thermal diffusivity of the liquid. The equation is solved using the implicit iterating method with 100 nodes in the r-direction.

Simulations have been carried out using both approaches (infinite conductivity and conduction limit), but no significant differences have been observed in the cases studied.

Correlation laws

To account for the influence of convection, linked to the instantaneous relative velocity of the droplet, we introduce correlation relations, both for mass and heat transfers. Following the film theory assumption [18], the non-dimensional vapour mass flow rate and vaporization Nusselt number are

$$\Lambda = \frac{Sh^*}{Le_l}\ln(1+B_M) \quad \text{and} \quad Nu = Nu^*\ln(1+B_T) \quad (7)$$

with

$$B_T = \frac{(T^\infty - T^s)C_{vap}}{q_g\pi D^2/\mathring{m}} \text{ (Spalding heat transfer number)} \quad (8)$$

where different correlation can be introduced in Sh^* and Nu^*, as mentioned by Renksizbulut and Haywood [7], Ranz and Marshall [19], Abramzon and Sirignano [18], and Faeth [3] following Fendell *et al.*'s [20] theoretical studies.

Since we are concerned here with small Reynolds numbers and small transfer numbers, results are quite constant whatever the correlation; the relation given by Faeth [3] is used

$$Nu^* = 2 + \frac{0.55\,Re^{1/2}\,Pr^{1/3}}{\left(1+\dfrac{1.232}{Re\,Pr^{4/3}}\right)^{1/2}}. \quad (9)$$

Assumptions for the equation of motion for evaporating droplets

Preliminary calculations have shown that the added mass term, pressure gradient term and Basset term were negligible in the equation of motion, which thus reads

$$\frac{d\mathbf{V}_p}{dt} = -\frac{3}{4}\frac{\rho_f}{\rho_l}\frac{C_D}{D}(\mathbf{V}_p - \mathbf{U})|\mathbf{V}_p - \mathbf{U}| + \mathbf{g} \quad (10)$$

where C_D is expressed through the Clift *et al.* [14] relation as far as the viscosity in the particle Reynolds number is estimated at a well defined reference state of temperature and vapour mass fraction ('1/3' rule [21]). C_D is thus expressed by

$$C_D = \frac{24}{Re}(1+0.15Re^{0.687}); \quad Re = \frac{|\mathbf{V}_p - \mathbf{U}|D}{\nu_{ref}}. \quad (11)$$

Miscellaneous remarks

Following the conclusions from Hubbard *et al.* [22], the physical properties of the gas phase are estimated in the gaseous film around the droplet, by using the averaging '1/3 rule'.

Let us mention that the assumption on the quasi-stationarity nature of the gas phase requires, as usual, a large fluid phase/gas phase density ratio [17], but also that the residence time of the droplet in the correlation domain defined in the Lagrangian approach is much greater than a characteristic diffusion time in the gaseous film (species molecular diffusion, for instance). In the present studies, for 100 μm droplets, this characteristic time is about 10^{-3} s, which is indeed much smaller than the Lagrangian integral time scale of the turbulence which is ranging from 5×10^{-2} to 10^{-1} s.

RESULTS

The respective influence of velocity, temperature or vapour mass fraction fluctuations is studied in isotropic and homogeneous turbulence. We have taken the grid turbulence data from Snyder and Lumley [23] for the turbulence field (vertical downwards flow with a mean velocity equal to 6.55 m s^{-1}, and classical decay laws for turbulence). Temperature and vapour mass fraction mean values and fluctuation intensities are assumed constant in the whole channel.

Methyl alcohol droplets are isokinetically injected 51 cm after the grid, and simulations are carried out until $X = 200$ cm from injection. The mean temperature is equal to 400 K and the mean vapour mass fraction is equal to 0.1. A great number of results have been obtained, but only the most significant are presented here.

Influence of velocity fluctuations

Great attention has been paid to the influence of velocity fluctuations on the droplet evaporation. This study is possible with the code PALAS which provides us with instantaneous quantities which are required for a good understanding of the phenomena. Most of the comparisons are between our Lagrangian simulations and results obtained without any influence of the turbulence, that means when the droplets are driven by the fluid mean properties only.

Calculations have been carried out for 10 000 trajectories and mean quantities are obtained by arithmetic averaging.

Figure 1 presents the reduced mean diameter D/D_0, where D_0 is the initial diameter of the droplets, vs the distance X from injection. Two initial diameters are considered, $D_0 = 100$ and 250 μm, and three cases for the turbulence, namely no turbulence, the standard u' decay law and a case where u' is arbitrarily multiplied by 2.

The influence of the turbulence on the mean diameter appears quite small, particularly for $D_0 = 250$ μm. The difference in the results for the two initial diameters is due to the different behaviour of the droplets, depending on the involved characteristic times:

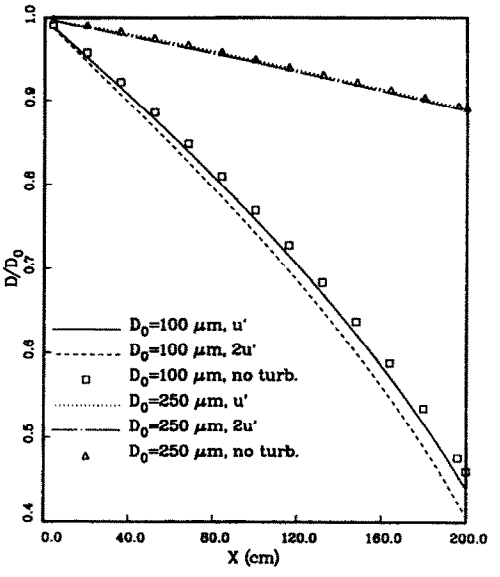


FIG. 1. Influence of velocity fluctuations on mean diameter.

(a) τ_p relaxation time of the droplet

$$\tau_p = \frac{(\rho_p + 1/2\rho_f)D^2}{18\mu};$$

(b) τ_L Lagrangian integral time scale;

(c) τ_c characteristic interaction time between fluid particle and droplet

$$\tau_c = \frac{\sqrt{(u'^2)}\tau_L}{\Delta U}.$$

Figures 2(a) and (b) present the three time scales for our particular case. We can observe that for 100 μm droplets, τ_P is smaller than τ_L and τ_C, but for 250 μm droplets τ_P is much greater than τ_C. These large droplets do not have time to react to the fluid fluctuations since, due to a quite large difference between their mean velocity and the fluid mean velocity, the interaction time between droplets and fluid particles is too small. Note that even without gravity (the same mean velocity for fluid and droplets) the influence of turbulence on the large droplets remains smaller than for small droplets, as τ_P is greater than τ_L which leads to an important loss of information exchange between fluid and particles.

Figure 3 presents the mean corrected Nusselt number Nu^* vs the distance from injection. As in Fig. 1, we can observe that the influence of the turbulence is more important on the smallest droplets. Note that the behaviour in the region near the injection is mainly due to initial conditions.

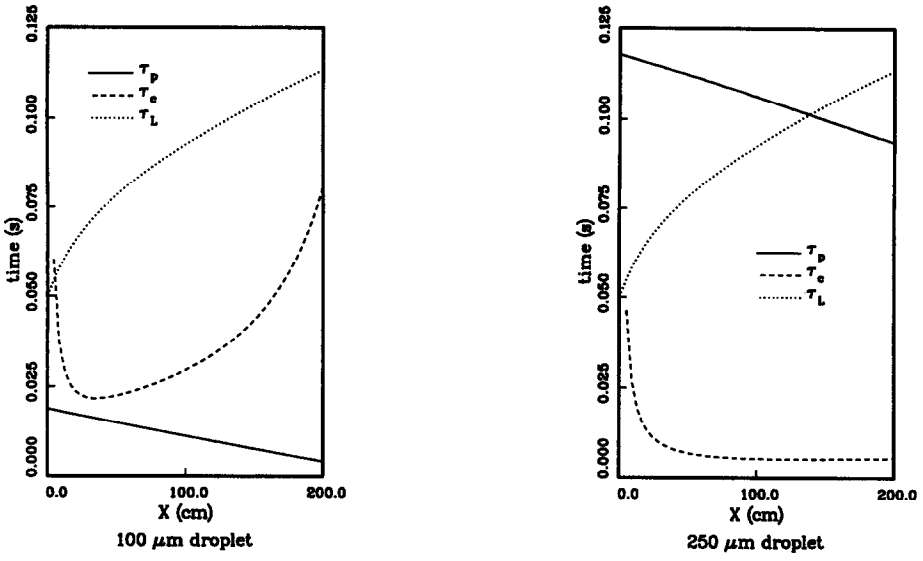


FIG. 2. Turbulence (a) and droplet (b) time scales.

The influence of fluctuating velocities on droplet diameters is shown in Fig. 4, where σ_D/D_0 is presented for the same cases as previously, where σ_D is the r.m.s. diameter. It can be observed that diameter distributions are broadening with X, as is obviously expected. We can also observe that the effect of turbulence on σ_D increases when diameters are decreasing, but also with a turbulence intensity increase (for $X = 200$ cm, $\sigma_D/D_0 = 0.010$ for u' and $\sigma_D/D_0 = 0.023$ for $2u'$). Nevertheless, this influence on the absolute r.m.s. values remains small (<1 μm for $X = 200$ cm and $D_0 = 100$ μm). For different turbulent flows, such as jets for example, turbulence intensities can be ten times higher than in grid turbulence, and the effect on absolute values should not be negligible.

Influence of temperature fluctuations

Two cases are considered, $T' = 10$ and 30 K, and the standard value of u' is kept in these simulations. As it can be observed in Fig. 5 the mean diameter is not affected by these temperature fluctuations. But the effect on the r.m.s. diameter appears as non-negligible as shown in Fig. 6 (between 3 and 10% of the initial diameter).

This behaviour is also observed on Fig. 7 where the pdf of the diameters is presented for $X = 200$ cm

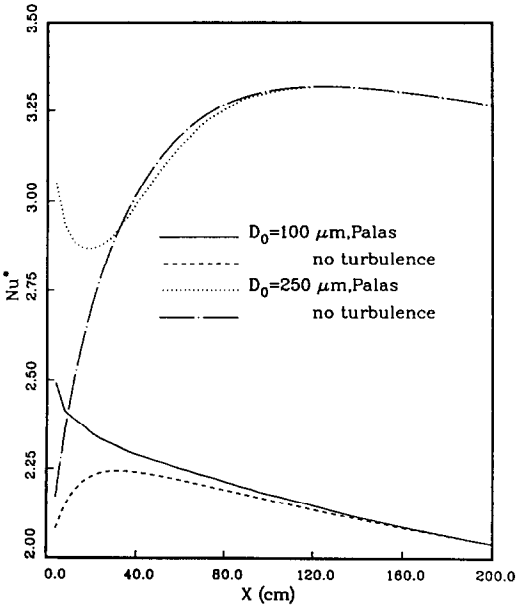


FIG. 3. Influence of turbulence on Nusselt number.

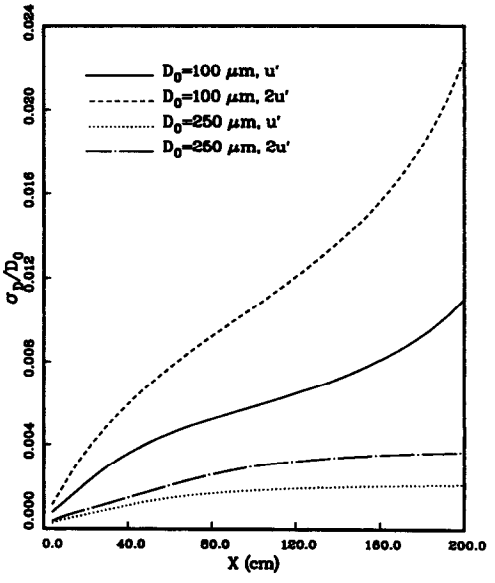


FIG. 4. Influence of velocity fluctuations on r.m.s. diameter.

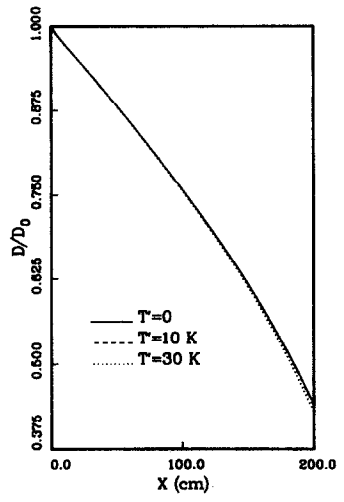


FIG. 5. Influence of temperature fluctuations on mean diameter.

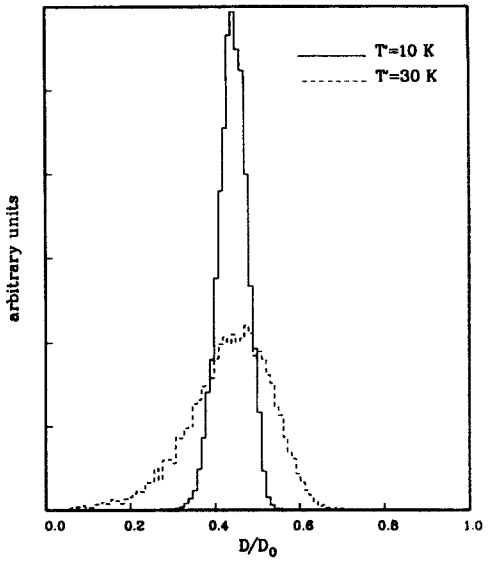


FIG. 7. Diameter pdf $X = 200$ cm for two temperature fluctuation intensities.

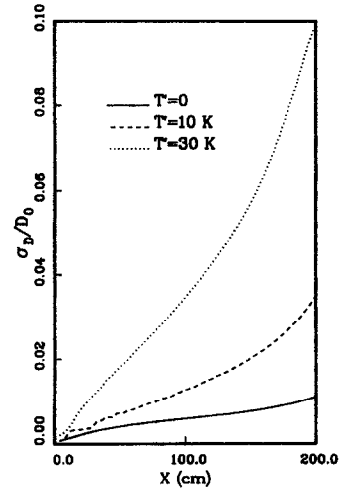


FIG. 6. Influence of temperature fluctuations on r.m.s. diameter.

from the injection, for the two different temperature fluctuations. When the fluctuation intensity increases, the pdf broadens, as expected, but, in addition, the symmetry of the profiles is lost. This simply results from the fact that dD^2/dt is approximately a constant, resulting in a bias towards smaller droplets: a pdf of D^2 instead of D would indeed be symmetrical. For $T' = 30$ K, broadening of the pdf is very significant: clearly this indicates that temperature fluctuations have to be considered when turbulent evaporation is studied.

Influence of vapour mass fraction fluctuations

As for temperature, two cases are considered, $Y' = 0.01$ and 0.02 (with no temperature fluctuations). No influence is observed on the mean diameters in both cases. The influence on the diameter distribution is presented on Fig. 8 where the r.m.s. diameter is shown vs X. The effects are very small, less than 0.5% of the initial diameter when compared with the result $Y' = 0$, that means with the velocity fluctuations only.

All fluctuations

The last results concern a case with the standard value for u', $T' = 30$ K, and $Y' = 0.02$. Figure 9 pre-

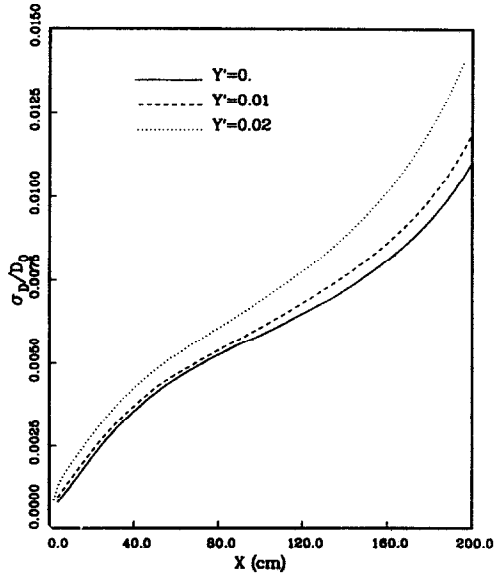


FIG. 8. Influence of concentration fluctuations on r.m.s. diameter.

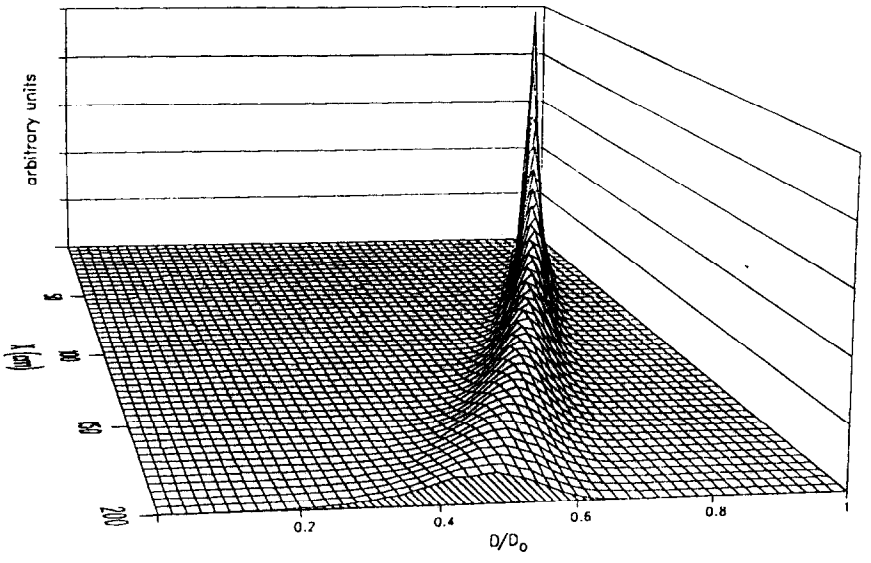


FIG. 9. Three-dimensional profiles of diameter pdf in grid turbulence.

sents the variation of the diameter pdf along the X-axis. As mentioned before, a dissymmetry appears in the profiles, due to turbulence effects. However, the most important result is the existence of such diameter distributions. When no turbulence is taken into account, diameters are represented through a peak which moves along the D/D_0 axis when X increases, without broadening.

CONCLUSION

A Lagrangian approach is used for the study of the influence of turbulence on droplet evaporation. Simulations are carried out in a grid turbulence and results are given for the respective influence of the fluctuating temperatures, fluctuating vapour mass fraction and fluctuating velocities, through the different variations of the mean diameter and diameter distributions.

In the studied case, influence of turbulence on the mean diameters remains small. However, an important result is the existence of diameter pdf which changes particle behaviours. The broadening of diameter distributions cannot be neglected, particularly when temperature fluctuations occur in the flow under study. Noting that turbulent intensities are small in grid turbulence compared with jets for example, the effects of turbulence on droplet evaporation must be included in simulations of such flows. Moreover, this influence has to be coupled with turbulent dispersion and the influence of particles on the turbulent field. New developments of the code are now planned for such complicated situations, but comparisons with experimental results must also be done, as soon as data becomes available from the literature.

Acknowledgements—The authors wish to acknowledge the Société Européenne de Propulsion for financial support in the presented research.

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SUR LA SIMULATION LAGRANGIENNE DE L'INFLUENCE DE LA TURBULENCE SUR L'EVAPORATION EN GOUTTELETTES

Résumé—Une approche lagrangienne est développée pour étudier l'influence de la turbulence sur l'évaporation de gouttelettes. Deux modèles peuvent être utilisés, conductivité infinie et limite de conduction. La convection est prise en compte par des corrélations où sont introduites des grandeurs fluctuantes de vitesse, température ou concentration. L'influence de la turbulence sur l'évaporation, pour la turbulence homogène, est discutée, les résultats étant aussi comparés avec des simulations qui concernent seulement des grandeurs moyennes.

SIMULATION DES TURBULENZEINFLUSSES AUF DIE VERDAMPFUNG VON TROPFEN IN DER BETRACHTUNGSWEISE NACH LAGRANGE

Zusammenfassung—Der Einfluß der Turbulenz auf die Verdampfung von Tropfen wird aufgrund der Betrachtungsweise nach Lagrange untersucht. Für die Beheizung der Tropfen werden zwei Modelle verwendet: eines mit unendlicher Leitfähigkeit und eines mit begrenzter Leitung. Die Konvektion wird durch Korrelationsgleichungen für die Schwankungsgrößen der Geschwindigkeit, der Temperatur oder der Konzentration berücksichtigt. Der Einfluß der Turbulenz auf die Verdampfung der Tropfen bei homogener Turbulenz wird diskutiert. Die Ergebnisse werden außerdem mit Simulationsrechnungen verglichen, die lediglich Mittelwerte berücksichtigen.

МОДЕЛИРОВАНИЕ ВЛИЯНИЯ ТУРБУЛЕНТНОСТИ НА ИСПАРЕНИЕ КАПЕЛЬ С ИСПОЛЬЗОВАНИЕМ МЕТОДА ЛАГРАНЖА

Аннотация—Методом Лагранжа исследуется влияние турбулентности на испарение капель. Для описания нагрева капель с бесконечной теплопроводностью могут использоваться две модели. Конвекция учитывается соотношениями, в которые входят флуктуации скоростей, температуры и концентрации. Обсуждается влияние турбулентности на испарение капель. Полученные результаты сравниваются с моделями, включающими только средние значения.