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THE ROLE OF NATURAL CONVECTION ON DROPLET EVAPORATION

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Abstract. *Evaporation of fuel droplets in high temperature gas environment is of great importance in many engineering applications. In practical situations, as well as in the majority of the experiments used for model validation, evaporating droplets are under normal gravity condition. Therefore, the incorporation of natural convection effects on the droplet evaporation rate by using an empirical correlation is investigated in the present study. The results of the numerical simulations reveal that taking natural convection effects into account by adding the Grashof number into the Ranz-Marshall correlation for Nusselt and Sherwood calculations overestimates the evaporation rate for droplet evaporation under atmospheric pressure when compared to experimental measurements. The effect of pressure on mass transfer is a combination between molecular diffusion and natural convection; therefore, it depends on the ambient temperature.*

Keywords: *Droplet evaporation, Natural convection, Grashof number, Numerical simulation*

1. INTRODUCTION

Evaporation of liquid droplets in high temperature gas environment plays an important role in technical applications, specially those involving spray combustion. Droplet evaporation under normal gravity condition is affected by natural convection. This phenomenon enhances energy and mass transfers between the evaporating droplet and the surrounding gas. Hence, depending on the ambient conditions, incorporating these effects might become essential to correctly predict droplet evaporation rate. The effect of buoyancy is even more important when predicting the evaporation of multicomponent fuel droplets (Habchi and Ebrahimian, 2012). The dimensionless Grashof number is a measure of free convective strength, representing the ratio of buoyancy to viscous force acting on a fluid. It is proportional to the square of the ambient pressure, p_g , and the cube of the droplet diameter, D_d .

Some experimental investigations have already been done to study the role of natural convection on droplet evaporation, such as Nomura *et al.* (1992), Hegseth *et al.* (1996), Kelly-Zion *et al.* (2009) and Verwey and Birouk (2018). Kitano *et al.* (2014) have also shown the need of considering natural convection effects even if the evaporation occurs under microgravity conditions. However, none of those studies have analysed the effect of introducing the Grashof number in the expressions of the Sherwood and Nusselt numbers by means of empirical correlations, which is the procedure usually used in numerical simulations. Hence, it is necessary to investigate if this method can accurately represent the natural convection contribution. The present study aims, first, to evaluate the role of natural convection on droplet evaporation under atmospheric pressure by comparing simulated results against experimental measurements; second, to analyse the effects of ambient temperature and pressure on natural convection and molecular diffusion as well as the total droplet evaporation rate; and, third, to verify the influence of the droplet initial diameter on the buoyancy effects.

2. EVAPORATION MODEL

Mass and thermal energy transfer processes are described by differential equations, which express the temporal changes of droplet size and temperature. The droplet mass variation throughout time is given by:

$$\frac{dm_d}{dt} = -\dot{m}_d, \quad (1)$$

where m_d is the droplet mass and \dot{m}_d is the droplet mass evaporation rate that leads directly to droplet size reduction:

$$\frac{dD_d}{dt} = -\frac{2\dot{m}_d}{\pi\rho_l D_d^2}, \quad (2)$$

where ρ stands for density and the subscript l refers to the liquid phase. The droplet temperature variation as a function of time is given by:

$$m_d c_{pl} \frac{dT_d}{dt} = Q_S, \quad (3)$$

where c_p is the specific heat capacity and Q_S is the power transferred to promote the droplet thermal energy variation per unit of time, which is transferred as heat.

Based on a detailed analysis of different evaporation models (Pinheiro and Vedovoto, 2018), the Abramzon-Sirignano evaporation model (ASM) (Abramzon and Sirignano, 1989) is adopted to represent the mass and energy transfers between the liquid and gaseous phases. In this model, the instantaneous droplet evaporation rate is given as:

$$\dot{m}_d = \pi D_d D_{vm} \rho_m Sh^*_m \ln(1 + B_M), \quad (4)$$

where D_v is the vapor diffusion coefficient, subscript m represents that the physical properties are evaluated at the gas-vapor mixture conditions in the film around the droplet determined by the 1/3 averaging rule (Ma *et al.*, 2016), Sh^* is the modified Sherwood number proposed by Abramzon and Sirignano (1989), and B_M is the Spalding mass transfer number, given by:

$$B_M = \frac{Y_{vs} - Y_{vg}}{1 - Y_{vs}}, \quad (5)$$

where Y_{vs} and Y_{vg} are the vapor mass fractions at the droplet surface and in the ambient gas far away from the droplet, respectively.

The vapor mass fraction at the droplet surface may be calculated using Raoult's law, which states that the surface vapor molar fraction, χ_{vs} , is equal to the ratio between the saturated vapor pressure, p_{vs} , and the ambient pressure, p_g :

$$\chi_{vs} = \frac{p_{vs}}{p_g}, \quad (6)$$

Therefore, once χ_{vs} is determined, Y_{vs} can be computed as:

$$Y_{vs} = \frac{\chi_{vs} W_v}{\chi_{vs} W_v + \chi_{gs} W_g}, \quad (7)$$

where W is the molecular weight, and subscripts v and g refer to the fuel vapor and the ambient gas, respectively.

Assuming that the temperature inside the droplet is uniform, the energy balance equation for the surrounding gas, coupled to Fourier's law for the convective energy transfer between gas and liquid as the surface boundary condition, yields the following expression for the sensible energy used to increase the liquid droplet temperature during the heat-up period:

$$Q_S = G \pi D_d Nu^*_m k_m (T_g - T_d) - L_v \dot{m}_d, \quad (8)$$

where k is the thermal conductivity, Nu^* is the modified Nusselt number, T_g is the ambient gas temperature and L_v is the latent heat of evaporation. The correction factor for energy transfer reduction due to the vapor diffusing out is:

$$G = \frac{\ln(1 + B_T)}{B_T}, \quad (9)$$

where B_T is the Spalding thermal energy transfer number.

$$B_T = (1 + B_M)^\varphi - 1, \quad (10)$$

where:

$$\varphi = \left(\frac{c_{pv}}{c_{pg}} \right) \left(\frac{Sh^*}{Nu^*} \right) \frac{1}{Le_m}, \quad (11)$$

where Le is the Lewis number:

$$Le_m = \frac{k_m}{c_{pm} D_{vm} \rho_m}. \quad (12)$$

Since $Nu^* = f(Nu)$ and $Sh^* = f(Sh)$, the Grashof number was incorporated in the Nusselt and Sherwood calculation to take into account natural convection effects. The evaluation of such non-dimensional numbers is given by Yuge (1960):

$$Nu = 2 + 0.6 \left[\max \left(Gr_d^{1/2}, Re_d \right) \right]^{1/2} Pr_m^{-1/3}, \quad (13)$$

$$Sh = 2 + 0.6 \left[\max \left(Gr_d^{1/2}, Re_d \right) \right]^{1/2} Sc_m^{-1/3}, \quad (14)$$

in which the droplet Grashof number, Gr_d , is defined as (Ebrahimian *et al.*, 2012):

$$Gr_d = \frac{g \rho_g^2 (T_g - T_d) D_d^3}{T_g \mu_m^2}, \quad (15)$$

Re_d is the droplet Reynolds number, Pr is the Prandtl number, Sc is the Schmidt number and μ is the dynamic viscosity.

ASM is implemented in the in-house code MFSim and it is used for the simulations in this work. The 4th-order Runge-Kutta scheme is used for the time discretization of Eqs. (2) and (3) to predict the temporal advancement of droplet size and temperature.

The physical properties for vapor and gas, identified with subscripts v and g , are obtained utilizing the open source Cantera software package (Goodwin *et al.*, 2016), based on the phase molar composition and reference temperature at the gas-vapor mixture, T_m . Furthermore, the diffusivity of fuel vapor in gas, D_{vm} , even when the gaseous phase is a mixture, is also directly calculated by Cantera as a function of molar composition, reference temperature and ambient pressure. Cantera computes the thermodynamic and transport properties based on the kinetic gas theory and the NASA database. In the present study, this database is provided by means of an input file from Cai *et al.* (2016). For more information on how Cantera computes those properties, the reader is referred to Sanjosé (2009).

The liquid droplet properties, ρ_l and c_{pl} , the latent heat of evaporation, and the saturated vapor pressure are calculated based on the database found in Green and Perry (1999). Finally, all the thermodynamic and transport properties for liquid, vapor and gas phases are assumed constant during each time step, but they vary from one time step to another due to the corresponding changes in droplet temperature.

3. RESULTS AND DISCUSSION

3.1 Evaporation model validation and evaluation of natural convection effects for different ambient temperatures

Figure 1 presents the squared non-dimensional diameter temporal evolution for numerical simulations performed with the Abramzon-Sirignano model without accounting for natural convection effects (ASM) and incorporating them (ASM*). As follows from comparing ASM and ASM* predictions, for all the tested ambient temperatures, incorporation of natural convection effects reduced the droplet lifetime, as expected. However, ASM* showed shorter droplet lifetime than the one measured in the experiment.

It can be verified from Fig. 2 and Eq. 15 that the droplet Grashof number decreases as the ambient temperature increases and it also decreases as the droplet diameter reduces. As the droplet evaporates, a progressive and rapid reduction in the droplet Grashof number is noticed. Figure 1 suggests that as the droplet diameter decreases, the validity of the empirical law to represent the natural convection effects may fail, since for all the tested cases ASM* predictions presented a noticeable agreement with experimental data in the beginning and then they diverge. Also, the ASM* predictions for intermediate ambient temperatures, 548 and 623 K, presented better agreement with experimental data, indicating that there might exist a droplet Grashof number range in which the empirical correlation used in this research fits better.

Figure 4 displays the area evaporation rate calculated from the data presented in Fig. 1. As it can be observed from Fig. 4, introducing natural convection effects by means of the empirical correlations presented in Eqs. 13 and 14 overestimates the evaporation rate obtained by the numerical simulations in comparison to the one measured experimentally for all the temperatures tested.

It is important to highlight that there might have several effects that could increase the experimental evaporation rate, as the ones already cited, but it is hardly arguable to find any external influence that could diminish it. Therefore, introducing natural convection effects in numerical simulations by Eqs. 13 and 14 might not correctly represent what really happens physically, at least not for the conditions evaluated in Fig. 1.

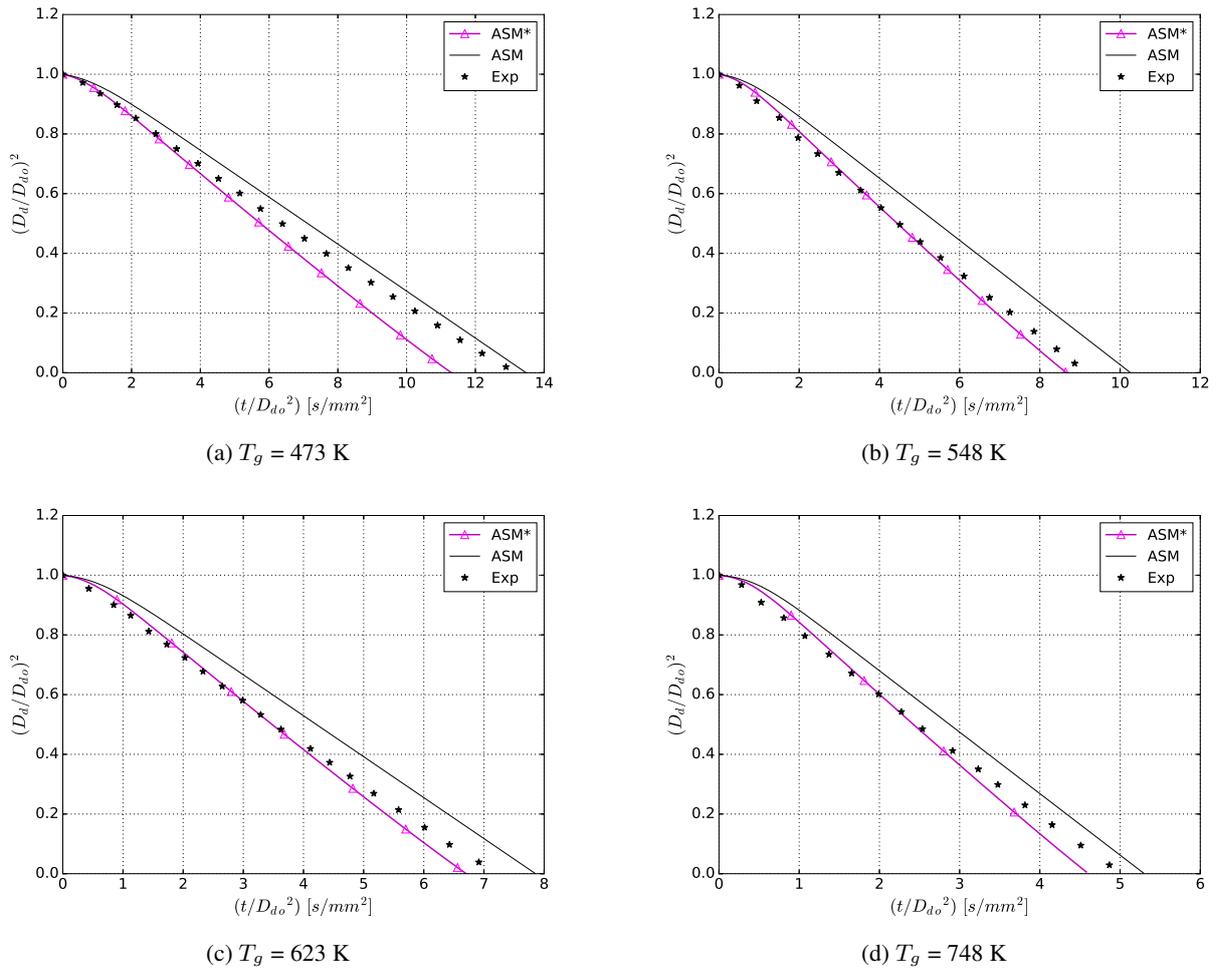


Figure 1: Variations of normalized squared droplet diameter with the time divided by squared initial droplet diameter with and without taking natural convection effects into account for n-heptane

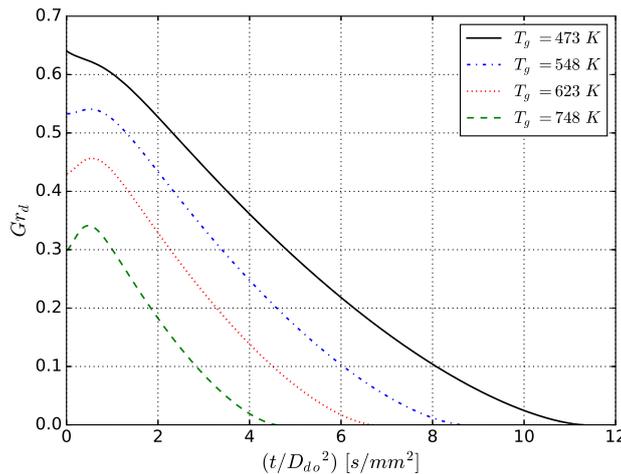


Figure 2: Temporal evolutions of droplet Grashof number for the ASM* predictions presented in Fig. 1 for n-heptane

3.2 Evaluation of natural convection effects for different ambient pressures

The evaporation rate of a droplet immersed in stagnant conditions at normal gravity is a function of natural convection and molecular diffusion. Pressure is expected to simultaneously improve natural convection and decrease molecular diffusion by suppressing the available molar fuel fraction on the droplet surface. Therefore, the natural convection effect on the droplet evaporation rate becomes more significant as the ambient pressure increases. Figure 2 and 4 shows the squared non-dimensional diameter temporal evolution for ASM with and without natural convection for different am-

bient pressures with gas temperature equals to 473 and 748 K. Figure 5 presents the area evaporation rate for both gas temperatures.

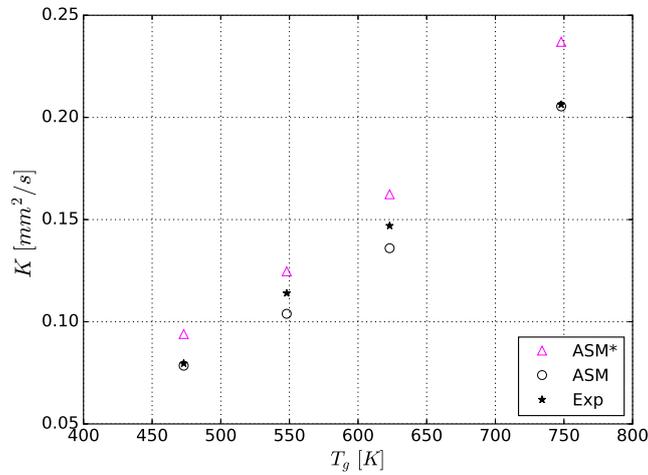
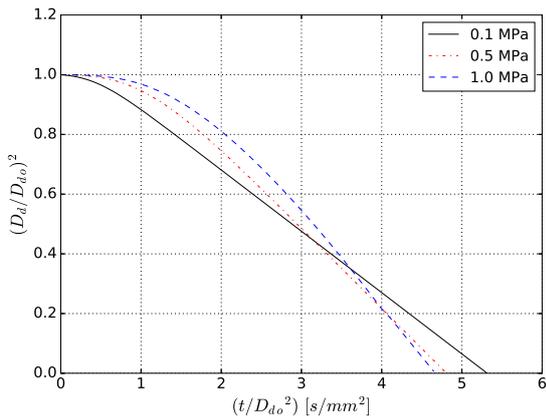
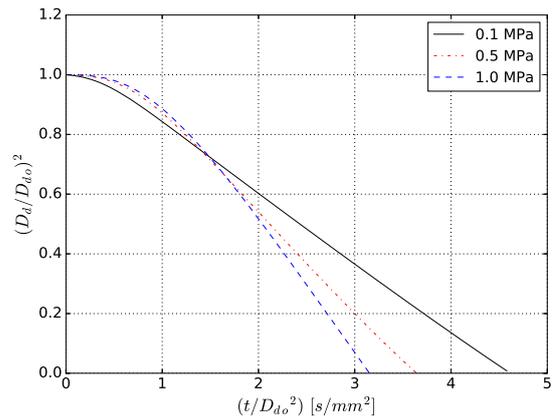


Figure 3: Comparison of the area evaporation rate, according to the ambient temperature, with and without taking natural convection effects into account for n-heptane

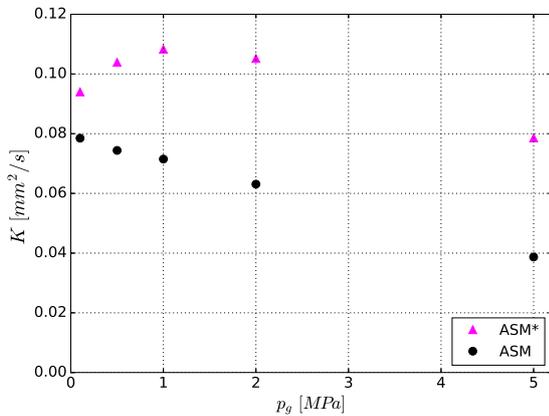


(a) Without natural convection

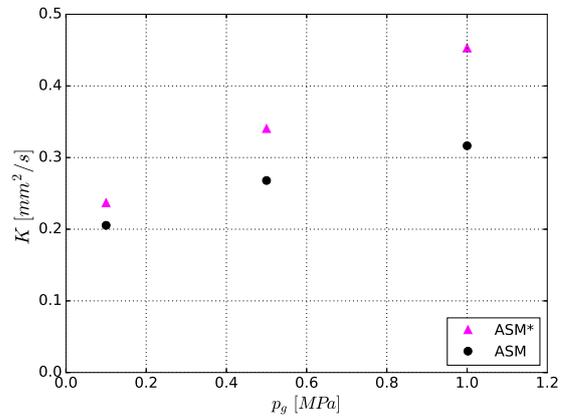


(b) With natural convection

Figure 4: Variations of normalized squared droplet diameter with the time divided by squared initial droplet diameter with and without taking natural convection effects into account for various ambient pressure and $T_g = 748$ K



(a) $T_g = 473$ K



(b) $T_g = 748$ K

Figure 5: Comparison of the area evaporation rate, according to the ambient pressure, with and without taking natural convection effects into account

Figure 5a shows two different behaviours for droplet evaporation under low temperatures. First, when natural convection is not considered, the evaporation rate monotonically decreases as the ambient pressure increases. It can be explained by the decline of available vapour molar fraction on the droplet surface, which reduces the molecular diffusion. On the other hand, when natural convection and molecular diffusion are considered together, the evaporation rate increases at first and diminishes for ambient pressures higher than 1.0 MPa. This happens because of those two competing effects. However, it is clear that natural convection effects increases with the ambient pressure since the difference in the evaporation rate between ASM and ASM* results is 16.49% for 0.1 MPa, but 50.76% for 5.0 MPa, as presented in Fig. 6.

Figure 5b, on the contrary, shows that for droplet evaporation under high ambient temperatures the evaporation rate increases, no matter if natural convection effects are taken into account or ignored. This observations reveals that the effect of ambient pressure on the evaporation rate of n-heptane droplets in fact depends on the gas temperature. Nevertheless, for the whole range of ambient temperatures tested, the natural convection effects increased with the ambient pressure, as shown in Fig. 6.

Even though introducing the Grashof number in the Ranz-Marshall empirical correlation overestimates the droplet evaporation rate for atmospheric pressure, this method might be useful for high-pressure cases since natural convection contribution becomes more remarkable. Therefore, there is a need of performing new experiments to study droplet evaporation under normal gravity at elevated ambient pressure using modern techniques in order to guarantee that no external heat source will affect the evaporation rate. This way it would be possible to evaluate if the use of Eqs. 13 and 14 actually allows incorporating the role of natural convection on droplet evaporation in high-pressure conditons.

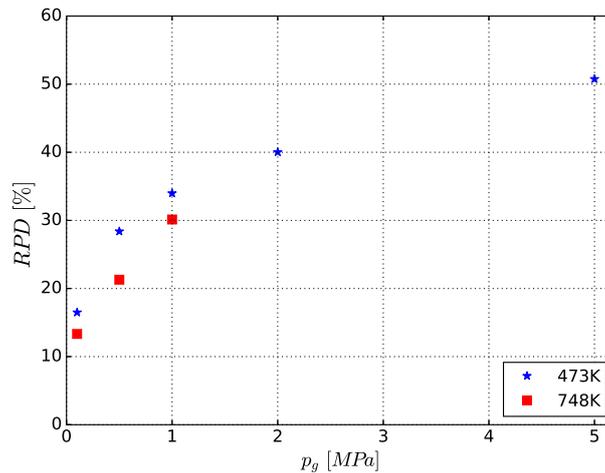


Figure 6: Relative percentage difference (RPC) between the area evaporation rate with and without taking natural convection, according to the ambient pressure

3.3 Evaluation of natural convection effects for different droplet initial diameters

Figure 7 presents the squared non-dimensional diameter temporal evolution for numerical simulations performed with the Abramzon-Sirignano model incorporating natural convection effects. As follows from comparing the histories for droplets with different initial size, for all the both tested ambient temperatures, incorporation of natural convection effects reduced the droplet lifetime more for bigger droplets, as expected. Since the Grashof number is proportional the cube of the droplet diameter, while the molecular mass diffusion is, theoretically, independent of droplet diameter, the relative importance of natural convection on the droplet evaporation rate is expected to increase with the initial droplet size. This behavior is indicated in Fig. 7 by the increasing area evaporation rate between initially small and large droplets.

4. CONCLUSIONS

In order to improve numerical simulation results, the incorporation of natural convection by means of the Ranz-Marshall empirical correlation was investigated. The use of the Grashof number as a way of incorporating natural convection effects with the traditional Ranz-Marshall empirical correlation for Nusselt and Sherwood calculation showed to overestimate the evaporation rate when compared with experimental data for atmospheric pressure. Therefore, this approach to take natural convection into account should be used carefully in order to avoid wrong droplet lifetime prediction, since it is usually used as a design parameter in engineering applications.

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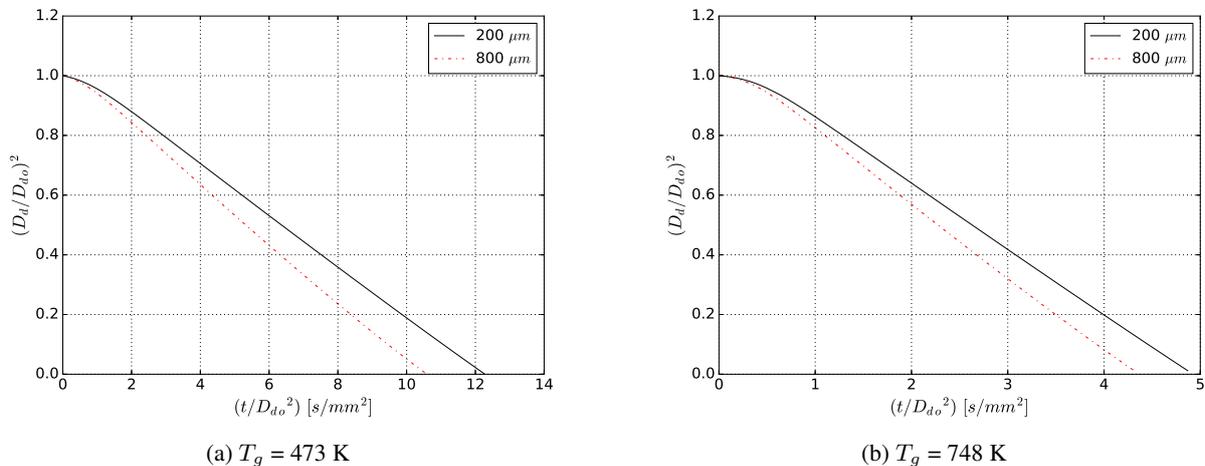


Figure 7: Variations of normalized squared droplet diameter with the time divided by squared initial droplet diameter taking natural convection effects into account for different droplet initial diameter

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