



# **The evaporation of a multicomponent fuel droplet at high pressure**

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## **Abstract**

The computer models used to calculate spray combustion are strongly dependent on the evaporation rate of the fuel droplets. Due to their complexity the droplet evaporation submodels are strongly simplified. This means that an unrealistic fuel composition is used (mono- or bicomponent fuel). The gas and liquid phases are usually treated as ideal, which is invalid at the high pressures that occur in the diesel engine. To explore the effects of these simplifications in detail, a realistic model of the evaporation of a single moving fuel droplet at high pressure is developed. In this paper the differential equations with their boundary conditions are presented and their numerical solution is discussed. It is shown that at a high pressure the evaporation rate is significantly different from the one of a steadily evaporating sphere with a constant radius, which is commonly used in models. Finally, to illustrate the model, results are shown for the evaporation of a gasoil droplet.

## **1 Introduction**

In recent years, a lot of work has been made on the modeling of diesel engine combustion. Because diesel engine combustion is a very complex combination of chemistry and two phase flow, the resulting computer codes are very extensive and complicated. For the time being, it is not possible to calculate the



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power cycle of a diesel engine accurately. Nevertheless, they can be very useful in giving insight in the relevant processes.

Because of the complexity of the subprocesses involved, simplified versions have to be used. One for practical reasons very unfortunate result of this is that the correspondence between an actual fuel and its representation - usually as a monocomponent fuel - is minimal. Also, because of the high pressures involved in the diesel engine, the ideal gas law becomes invalid and this is usually not taken into account. This limits the insight that can be gained from these models.

For these reasons, a single moving droplet evaporation model was developed. This model is demonstrated here for the evaporation of a droplet consisting of an automotive gasoil (represented as a mixture of 10 components), for conditions equivalent to those present in a diesel engine at the start of injection.

### 2 Description of the evaporation of a single droplet

Inside and outside the droplet, several different processes occur simultaneously (see figure 1). Because of the high gas temperature, the fuel starts to evaporate at the surface. The resulting vapor is convected away from the surface by the gas flow surrounding the droplet. Because the different fuel fractions evaporate at different rates, the composition of the droplet changes at the surface. The resulting internal concentration gradients cause diffusion within the droplet. At the same time heat conduction from the hot surface will raise the temperature inside the droplet. Due to drag, the relative velocity between droplet and gas will gradually decrease. Heat and mass transfer between the gas and the liquid phase are influenced by the Stefan flow perpendicular to the surface, caused by the evaporation. Internal flow, caused by friction at the surface of the droplet, will enhance transport within the droplet. All these phenomena are modeled to calculate the droplet evaporation accurately.

Because the droplet radius changes as the evaporation proceeds, the problem has a moving boundary.

The surface tension of the fuel causes the droplet to stay nearly spherical throughout its lifetime. For simplicity spherical symmetry of temperature and composition in the droplet interior is assumed. The processes outside of the sphere are modeled as quasi-stationary.

### 3 Detailed description of the different submodels

#### 3.1 Vapor-liquid equilibrium

The vapor-liquid equilibrium calculation is complicated by the fact that during its lifetime the droplet surface will reach a temperature higher than the critical temperature of some of its components. This means that the law of Raoult (Reid<sup>1</sup>) can't be used because the vapor pressure of a liquid hotter than its

critical temperature is undefinable. Because of the high pressure in a diesel engine, the behavior of the vapor phase deviates very significantly from that of an ideal gas, and liquid properties become dependent of pressure. Therefore the ideal gas law is replaced by the real gas law :

$$Z = \frac{pV}{RT} \quad \text{with} \quad Z = Z(p, T)$$

which is modeled using a cubic equation of state :

$$Z = \frac{pV}{V-b} - \frac{a}{V^2 + u b V + w b^2}$$

There are several versions of the cubic equation of state (different choices for  $a$ ,  $b$ ,  $u$  and  $w$ ), that are named after the author(s) who developed them (van der Waals, Redlich-Kwong, Soave and Peng-Robinson). For detailed descriptions the reader is referred to Reid, Prausnitz & Poling<sup>1</sup> : together with a mixing rule that describes  $a$  and  $b$  as a function of the  $a$ 's and  $b$ 's of its components, this equation of state can be used to calculate not only volumetric properties, but also the vapor-liquid equilibrium and the required thermodynamical properties like the specific heats and the latent heat of vaporization.

### 3.2 Droplet deceleration

The classic equation of motion is given by :

$$\bar{F} = m \frac{d\bar{v}}{dt} = - C_D \frac{\pi d^2}{4} \frac{1}{2} \rho \left| \bar{v} - \bar{v}_{gas} \right| (\bar{v} - \bar{v}_{gas})$$

Since the deformation of the droplet is negligible during most of its lifetime, the drift coefficient for solid spheres can be used. The influence of heat and mass transport is small and can be taken into consideration by using appropriate values of the transport parameters. This is done by using the 1/3 rule (Yuen & Chen<sup>2</sup>). The drift coefficient is best represented by the formula of Langmuir (Putman<sup>6</sup>) :

$$C_D = \frac{24}{Re} (1 + 0.197 Re^{0.63} + 0.00026 Re^{1.38})$$

If the gas velocity is assumed to be constant, the relative velocity of the droplet will rapidly decrease to zero. This will not happen in reality because of the turbulence in the cylinder. Since the convective transport of heat and fuel vapor depends strongly on this relative velocity, it is best to assume a fluctuating gas velocity. In this work it was chosen to model the gas velocity as a vector with constant magnitude, rotating with constant frequency. This gas velocity will (after an initial deceleration) lead to a terminal droplet velocity with the same characteristics (if the droplet diameter is kept constant).



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However, during the transient deceleration phase, the gas velocity is set to zero because otherwise fluctuations with frequency  $f$  would complicate interpretation of the results. The non-zero gas velocity is introduced at the point where the droplet velocity is equal to its terminal velocity. Afterwards the droplet velocity stays equal to the terminal velocity (which only changes because of the reduction of the diameter of the droplet).

### 3.3 Heat and mass transfer outside the droplet

The convection around a solid moving sphere is determined by (Faeth<sup>3</sup>):

$$\text{Nu} = 2 + \frac{0.555 \text{Re}^{1/2} \cdot \text{Pr}^{1/3}}{\sqrt{1 + \frac{1.232}{\text{Re} \cdot \text{Pr}^{4/3}}}}$$

If the evaporation at the fuel droplet is not too fast, the mass transfer is similar to the heat transfer. Therefore, a formula analogous to that for heat transfer is to be used for each component  $i$  (Faeth<sup>3</sup>):

$$\text{Sh}_i = 2 + \frac{0.555 \text{Re}^{1/2} \cdot \text{Sc}_i^{1/3}}{\sqrt{1 + \frac{1.232}{\text{Re} \cdot \text{Sc}_i^{4/3}}}}$$

In these formulas the gas properties must be evaluated according to the 1/3 rule (Abramzon & Sirigano<sup>7</sup>).

Since the evaporation at the surface influences the heat transfer because it introduces a blowing effect perpendicular to the surface (Stefan flow), the filmtheory correction must be used to get accurate results. This is described in section 4.

### 3.4 Heat transport within the droplet

The heat equation within the droplet is given by (Bird, Stewart & Lightfoot<sup>4</sup>) :

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \cdot \nabla T)$$

The values of  $c_p$  and  $\lambda$  depend on the distance from the center, because the temperature gradient is considerable and both parameters are function of temperature. We must combine this with the boundary condition :

$$\lambda \left. \frac{dT}{dr} \right|_{r=R} = \dot{q}_s = h^*(T_\infty - T_s) - \sum_i \dot{m}_i h_i^{ev}$$

in which the evaporative mass flux equals :

$$\dot{m}_i = k_i^* \rho_i^{\text{vap}} + \rho_i^{\text{vap}} \left| \frac{dR}{dt} \right|$$

The first term is the convection/diffusion term (relates to the total mass flux at a certain location), the second is due to surface regression.

### 3.5 Mass transport within the droplet

Due to the difference in evaporation rate for the different components, the droplet composition at the surface will deviate from the composition at the center. This will gradually cause diffusion within the droplet. The mass flux due to diffusion is given by the law of Fick (Reid, Prausnitz & Poling<sup>1</sup>; Bird, Stewart & Lightfoot<sup>4</sup>):

$$\dot{J}_i = -D_i \nabla \rho_i$$

If the diffusion rates of the different species are not identical, this equation suggests that net mass flow will occur. To maintain isobaric conditions in the liquid however, bulk motion of the mixture will be generated. If such a bulk motion is introduced, the diffusion equation becomes:

$$\frac{\partial \rho_i}{\partial t} = \nabla(D_i \nabla \rho_i) - \nabla(\rho_i v_b)$$

For the liquid hydrocarbon mixtures that are relevant here, the density varies only slightly with composition. We therefore determine the bulk velocity by keeping the density constant. This leads to the result:

$$\frac{\partial \rho_i}{\partial t} = \nabla(D_i \nabla \rho_i) - \frac{1}{\rho} \nabla \left( \rho_i \sum_j D_j \nabla \rho_j \right)$$

The corresponding boundary condition at the surface of the droplet is (see figure 2):

$$D_i \left. \frac{\partial \rho_i}{\partial r} \right|_{r=R} - \frac{\rho_i}{\rho} \sum_j D_j \left. \frac{\partial \rho_j}{\partial r} \right|_{r=R} = (\rho_i - \rho_i^{\text{vap}}) \left| \frac{dR}{dt} \right| - k_i^* \rho_i^{\text{vap}}$$

### 3.6 Surface regression

Due to the evaporation of fuel from the droplet, its radius will decrease continuously. By summing the evaporation fluxes we obtain:

$$\left| \frac{dR}{dt} \right| = \frac{\sum_i k_i^* \rho_i^{\text{vap}}}{(\rho - \rho^{\text{vap}})}$$



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Since the boundary conditions of the partial differential equations are given at a moving surface, the equations described above are not practical in this form. Therefore the differential equations are written for a grid that is connected with the droplet surface. This is described in section 5.

### 3.7 The effect of liquid motion

It is well known that the friction with the surrounding air induces a circulating flow within the droplet. This flow field - usually referred to as the Hill-vortex - enhances mixing in the liquid phase. For one-dimensional models the effect thereof can be modeled by multiplying the thermal conductivity and the internal diffusion coefficients with an appropriate constant factor, as shown by Abramzon & Sirigano<sup>7</sup>.

Very rapid mixing does not lead to a homogeneous temperature and composition inside the droplet: the nature of the flow field will cause the center of the droplet to have nearly the same properties as the surface, but gradients perpendicular to the streamlines stay present.

## 4 The boundary conditions in the gas phase

The evaporation of the fuel molecules at the surface of the droplet generates the Stefan flow perpendicular to the surface, because of the volume difference between liquid and vapor. This flow field will influence both heat and mass transfer. The film theory provides the appropriate background to calculate these effects (Bird, Stewart & Lightfoot<sup>4</sup>).

The resulting equations are so extensive that they won't be represented here: the reader is referred to Rossee<sup>5</sup>. To get some insight in the results however, we will look at the special case of the monocomponent fuel droplet. In this case the molar evaporative fluxes reduce to:

$$\dot{n} = \left( k^* + \left| \frac{dR}{dt} \right| \right) n_F = k^* \left( 1 + \frac{x_F}{\beta - x_F} \right) n_F = k \frac{\ln \left( 1 + \frac{x_F}{1 - x_F} \left( 1 - \frac{1}{\beta} \right) \right)}{1 - \frac{1}{\beta}} n$$

with:

$$\beta = \frac{\rho^{\text{liq}}}{\hat{\rho}^{\text{vap}}} \quad \text{and} \quad \hat{\rho}^{\text{vap}} = \frac{pM}{ZRT}$$

Because the liquid densities of all liquid fuels are nearly the same,  $\beta$  is mainly a function of the molecular weight, pressure and temperature. This means that - for the very high pressures occurring in the diesel engine - special behavior occurs. This will be even more pronounced for heavier fuels (higher molecular weights).

It is easily seen that for a small molar fuel fraction at the surface  $x_F$  the correct solution is obtained. Also, if the liquid density is much higher than the vapor density, the classical solution for the non-evaporating sphere (constant radius) is obtained.

Near the critical point (where  $\beta$  becomes 1) the correct singularity for  $x_F = 1$  is obtained. In this case phase transition can occur without the necessity of diffusion ( $k$  can be 0).

To get an idea of the inaccuracies that are introduced when the surface regression is assumed, we look at how different the evaporation rates can be compared with the - very often used - case of the steadily evaporating sphere. As can be seen in figure 3, for high  $x_F$  the effect should not be neglected.

## 5 The solution of the partial differential equations

The diffusion and heat equations inside the droplet can be written easily for spherical symmetry. To remove the moving boundary at the surface, we formulate the problem in the space coordinate  $r/R$  (Crank<sup>8</sup>). Although the procedure is straightforward, very complex equations result, for which the reader is referred to Rosseel<sup>5</sup>. The linear PDE's that result contain coefficients that are function of  $R$  and  $dR/dt$ , and therefore depend on the complicated boundary conditions at the surface. For the numerical solution the McCormack version of the Lax-Wendroff discretisation was chosen, because it is an explicit method. These explicit methods have the advantage that the coefficients of the PDE's don't have to be estimated at future times, which would complicate things here because of the complexity of the vapor-liquid equilibrium equations.

The grid used for the discretisation is adapted to the numerical solution of the differential equations, because this allows us to take account of the steep gradients at the surface at the start of the calculations (Rosseel<sup>5</sup>).

## 6 Some simulation results

When the droplet enters the combustion chamber, it heats up at its surface. Because the droplet decelerates gradually, and because of the increasing evaporation at higher temperatures, this temperature increase slows down. The temperature at the center of the droplet also increases, by internal conduction. It can be seen from figure 4 that temperature differences within the droplet are very significant.

The evolution of the droplet radius is shown in figure 5. It shows very clearly that evaporation occurs at an ever increasing rate.

In figure 6 we see the variation in the total fuel fraction in the vapor layer at the surface of the droplet. The continuous increase is caused by ever higher temperatures. Contrary to commonly used assumptions, approximately constant conditions are never reached.

The difference in evaporation rate at the surface causes a change in surface composition. As is seen from figure 7, because of diffusion within the droplet, this influences the concentrations throughout the droplet.

In figure 8 and 9, a comparison is shown between the standard calculation and a model in which the liquid properties (conductivity, specific heat, diffusion



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coefficients, ...) are independent of location. As can be seen clearly, this has a large effect on the calculation results. These assumptions are therefore not acceptable if accurate results must be obtained, although they are very often used.

### Conclusions

A mathematical model was developed for the calculations of the evaporation of a realistic fuel droplet at high pressure and temperature. This model is applicable for the case of the diesel engine.

This model is significantly different from others because of the special method used for the calculation of liquid/vapor equilibrium, the correct application of the film theory correction for transport in the vapor phase with surface regression and the true multicomponent character of the fuel (especially with respect to the modeling of the diffusion within the droplet).

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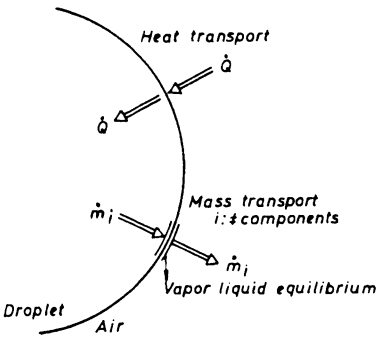


Figure 1: The evaporating droplet.

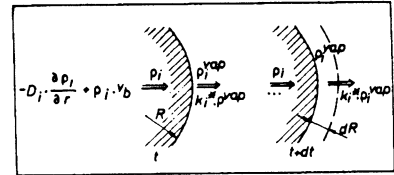


Figure 2: The boundary condition.

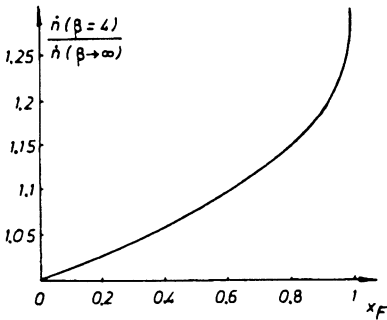


Figure 3: The influence of the surface regression.

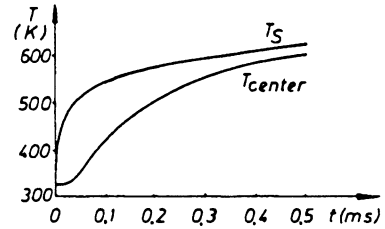


Figure 4: The evolution of the temperatures.

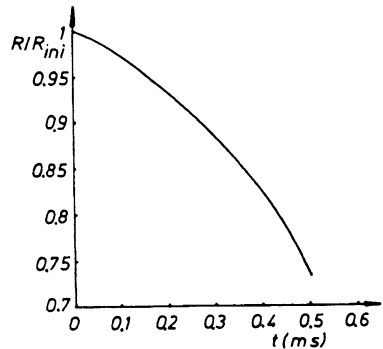


Figure 5: The evolution of the droplet radius.



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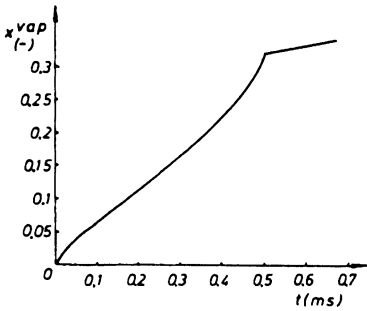


Figure 6: The evolution of the vapor phase.

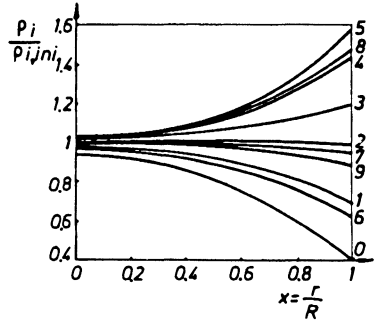


Figure 7: The concentration profiles.

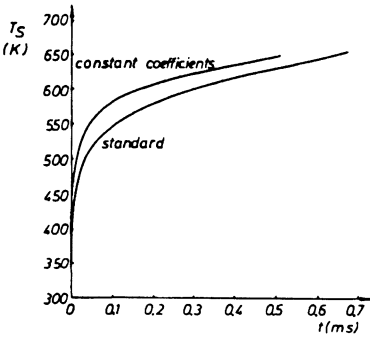


Figure 8: The importance of variable coefficients.

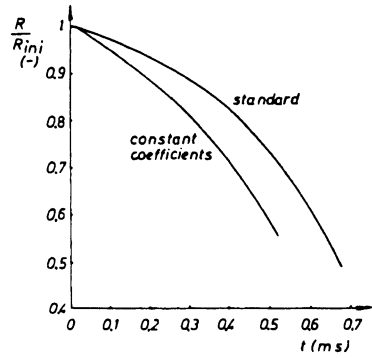


Figure 9: The importance of variable coefficients.



# Continuous casting: a front tracking Boundary Element Method solution

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## Abstract

The heat transfer problem in an ingot during continuous casting is discussed. Steady state temperature field in a co-ordinate system attached to the mould has been considered. Phase change is assumed to take place at constant temperature. The nonlinearity in this problem is caused by the unknown location of the solid liquid interface. To determine both this location and the temperature field in the ingot an original BEM technique has been developed.  $C^1$  smooth quadratic elements has been used to interpolation of phase change interface. Finally, the interface has been approximated by Bezier cubic splines to decrease the number degrees of freedom of this interface. A numerical example is included and discussed.

## 1. Introduction

The continuous casting process of metals and alloys is nowadays frequently utilized in metal industry. The scheme of this process is shown in Fig. 1. The liquid metal inflows into the mould (crystallizer) having the walls cooled by water. The ingot is pulled out by the withdrawal rolls. The solidification process starts in the mould. Below the mould the ingot surface is very intensively cooled by the spraying water outflowing from this mould.

There are number of reasons causing, that mathematical modelling of the temperature distribution in the ingot during continuous casting is a very challenging task. What follows are the main of them:

1. position of the phase change boundary, where heat generation takes place as a result of the liquid - metal solidification, is unknown. This position has to be determined while the temperature distribution problem in the ingot is solved,