Implementation of a new and improved evaporation model in Fluent

Thomas Vik and Bjørn Anders Pettersson Reif

Norwegian Defence Research Establishment (FFI)

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Approved by

Monica Endregard	Project Manager
Jan Ivar Botnan	Director

English summary

The release and dispersion of toxic chemicals can cause a threat to military personnel and the population at large. In order to develop and implement appropriate protective capabilities and plan mitigating measures, modelling, simulation and assessments of hypothetical scenarios and historical incidents is a valuable and widely used methodology. This requires reliable CBRN modelling and simulation capabilities for modelling how toxic chemicals are released and dispersed in air. A physical and mathematical model of an event involving the dispersion of chemicals can roughly be divided into three parts: source modelling, transport modelling and effect modelling. This study focuses on source modelling.

As part of the recent NATO-study SAS-061, research groups in the U.S., The Netherlands and FFI assessed the same scenario involving release of the chemical warfare agent (CWA) sarin. The groups used evaporation rates for sarin which varied by a factor of 10. This leads to correspondingly large variations of the calculations of the consequences and the extent of damage. This introduces an unacceptable uncertainty in consequence assessments and clearly demonstrates the need to improve our fundamental knowledge of evaporation processes.

This report describes the integration of an analytical evaporation model in computational fluid dynamics (CFD) software. Numerical simulations of the evaporation from droplets and the subsequent transport of vapour in a turbulent air field is conducted. The evaporation rate obtained in the numerical simulations is compared with the rates calculated analytically. The model is in addition compared with results obtained with other evaporation models used for CFD. The model is an substantially improvement to the default evaporation model in Fluent.

Sammendrag

Utslipp og spredning av giftige kjemikalier kan utgjøre en trussel mot militært personell og befolkningen i allmennhet. Modellering, simulering og analyse av hypotetiske scenarier og historiske hendelser en svært verdifull og mye brukt metode for å utvikle og implementere passende beskyttelseskapabiliteter og planlegge beskyttelses- og mottiltak. Dette krever at prosesser der giftige kjemikalier slippes ut og spres i luft kan modelleres og simuleres på en troverdig måte. En fysisk og matematisk modellering av en spredningshendelse kan grovt sett deles inn i tre deler: kildemodellering, transportmodellering og effektmodellering. Denne studien tar fokuserer på kildemodellering.

I en NATO-studie nylig gjennomført, SAS-061, analyserte forskningsgrupper i USA, Nederland og FFI hver for seg et scenario som involverte spredning av det kjemiske trusselstoffet sarin. De ulike gruppene benyttet fordampingsrater som varierte med en faktor 10. Dette medfører tilsvarende store variasjoner i beregninger av konsekvenser og skadeomfang. Dette gir en uakseptabel usikkerhet i konsekvensvurderingene og demonstrerer nødvendigheten av å forbedre vår fundamentale kunnskap om fordampingsprosesser.

Denne rapporten beskriver integrering av en analytisk fordampingsmodell i et dataverktøy for numeriske beregninger av strømning. Numeriske simuleringer av fordamping fra dråper og transport av den resulterende dampen i en turbulent luftstrøm er gjennomført. Fordampingsraten i de numeriske beregningene er sammenlignet med fordampingsrate beregnet analytisk. I tillegg er modellen sammenlignet med fordampingsmodeller brukt for numeriske beregninger. Modellen er en vesentlig forbedring til Fluent sin standard fordampingsmodell.

Contents

1 Introduction

The release and aerial dispersion of toxic chemicals, both as a result of accidents or willful actions, may pose a threat to military personnel and the population in general. Modelling, simulation and assessment of hypothetical scenarios and historical incidents is a valuable tool for developing and implementing appropriate protective capabilities and plan mitigating measures. This requires reliable CBRN modelling and simulation capabilities for modelling how toxic chemicals are released and dispersed in air. A complete model for an event involving the dispersion of a toxic chemical can roughly be divided into three parts: source modelling, transport modelling and effect modelling[1]. The present study concerns source modelling.

In the recent NATO-study SAS-061 [2], a scenario involving the release of the chemical warfare agent (CWA) sarin were assessed by research groups in the U.S., The Netherlands and FFI. The different groups used evaporation rates which varied by a factor of 10. This uncertainty about the true evaporation rate introduces an unacceptable uncertainty in consequence assessments and clearly demonstrates the need to improve our fundamental knowledge of evaporation processes.

An analytical model for the evaporation from a thin liquid surface beneath a turbulent boundary layer was developed at FFI [3]. This model is from here on referred to as FFI model. The present report concerns the integration and testing of the model in computational fluid dynamics (CFD) software. The analytical model is also compared with other evaporation models.

The analytical model and computational fluid dynamics in general is briefly considered in chapter 2. The numerical simulations are presented in chapter 3 and the results in chapter 4. In chapter 5 the model is compared against other evaporation models. Finally chapter 6 gives the conclusions and plans for further work.

2 Background

2.1 Evaporation models

2.1.1 FFI model

An analytical evaporation model developed at FFI is presented in [3]. A brief summary is given here. The model describes the transport of vapour through a turbulent boundary layer. The model does only indirectly take account for thermal effects. It is also assumed that the vapour resulting from the evaporation process can be treated as passive, that is the vapour does not influence the ambient air stream. This is not true; a study by Desoutter *et al*. [4] studied the impact of density differences between the vapour and air, and showed that it is significant. It is planned to extend the model to include these effects. At the present time, the model is valid for liquids with a relatively high boiling point, like typical chemical warfare agents or water, as thermal effects otherwise would have to be more accurately accounted for.

In the model, the concentration of vapour above the liquid surface as function of the friction velocity, u_*, and time, t, is calculated as:

$$C(u_*, t) = C_0 \mathcal{G} \frac{u_*}{\nu} \exp\left(-\mathcal{H} t^2\right) \tag{2.1}$$

where ν is the kinematic viscosity of air, C_0 the saturation concentration of the chemical and $\mathcal{G}$ and $\mathcal{H}$ model coefficient (see [3] for details). A mass flux is then calculated as:

$$F = v_{vap} A_0 \int_0^\tau C dt \tag{2.2}$$

where the vapour flux velocity v_{vap} is taken to be the mean streamwise velocity in the linear sub-layer, and the area A_0 to be the area of a plane span out by the droplet and the height of the linear sub-layer[1].

2.1.2 Default Fluent evaporation model

Fluent includes an evaporation model for the Discrete Phase Model. This model is based on gradient diffusion. A molar flux of evaporated vapour from a surface is calculated as:

$$N_i = k\left(C_{i,s} - C_{i,\infty}\right) \tag{2.3}$$

where $C_{i,s}$ is the concentration at the surface (equal to the saturation concentration at the current temperature), $C_{i,\infty}$ is the concentration in the bulk gas (which is known from the solution), and the mass transfer coefficient is given by the Sherwood number:

$$Sh = \frac{kd}{D} = 2.0 + 0.6 Re_d^{1/2} Sc^{1/3} \tag{2.4}$$

where d is the droplet diameter, D the diffusion coefficient, Re_d the Reynolds number based on the particle diameter and the relative velocity between the particle and the ambient air field, and $Sc = \mu/(\rho D)$ the Schmidt number. In addition, Fluent calculates the heat transfer to/from the droplets.

This law is designed to model evaporation from airborne droplets. In this work however, droplets impinged on a surface is considered. When computing Re_d it is assumed that the droplets stays at rest on the surface.

2.1.3 NSWCDD models

Naval Surface Warfare Centre Dahlgren Division (NSWCDD) in USA have created two different evaporation models for use in CFD calculations: hybrid and ADVEDS.

The hybrid evaporation model is similar to the default Fluent model with the exception of some model parameters:

$$\frac{\Delta m}{\Delta t} = \pi r_s D Sh\left(C_0 - C\right) \tag{2.5}$$

[1]There is another version of the model where the vapour flux velocity is taken to be the friction velocity and the area to be the surface area of the droplet.

where r_s is the surface droplet contact radius, C_0 the saturation concentration and C the concentration in the bulk gas. They have the following equation for the Sherwood number:

$$Sh = 0.0365 Re^{0.8} Sc^{0.62}. \tag{2.6}$$

where the Reynolds number is based on the surface droplet contact radius and the slip velocity between the droplet and the air stream. The surface radius is assumed constant, giving a constant evaporation rate.

The ADVEDS model calculates the evaporation by the equation:

$$\frac{\Delta m}{\Delta t} = k 2\pi r_{av} h \rho_{liq} \tag{2.7}$$

where r_{av} is the mass average radius of curvature for the droplet, h the droplet surface height and ρ_{liq} the liquid density. The mass transfer coefficient is given as:

$$k = 3.0557 \cdot 10^{-10} + \frac{0.076932 C_0 \left(100 v_s\right)^{0.55}}{100 \rho_{liq}} \tag{2.8}$$

where v_s is the slip velocity. Also for this model, the surface radius is kept constant. However the droplet height changes in time. The volume of the spherical cap is given by:

$$V = \frac{1}{6}\pi h \left(3r^2 + h^2\right) \tag{2.9}$$

By taking the time derivative, the following expression can be found for the height of the droplet:

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{-2\dot{m}}{\rho\pi\left(r^2 + h^2\right)} \tag{2.10}$$

where $\dot{m}$ denotes the time derivative of mass (in other words the evaporation rate). In addition, the average curvature changes in time.

2.2 Computational Fluid Dynamics

2.2.1 Turbulent flows

The flow of a Newtonian fluid is described by the Navier-Stokes equations, which accounts for the conservation of momentum and mass. For an incompressible flow these are:

$$\rho\left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right) = -\frac{\partial p}{\partial x_i} + \mu\left(\frac{\partial^2 u_i}{\partial x_j^2}\right) + f_i \tag{2.11}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2.12}$$

where ρ is the density, u_i the velocity components, t time, x_i the spatial coordinates, p the pressure, μ the dynamical viscosity and f_i outer forces (like e.g. gravity). These equations are valid for both turbulent and laminar flows. For turbulent flows however, the equations do not have an analytical solution, and must be solved numerically.

In order to solve the equations numerically, one common method is the finite volume method. In this method a computational mesh, which is a representation of the computational domain by small cells, is created. The equations are then solved in each of these cells. The calculated variables are localised in the centre of the cells, and it is assumed that the variable does not change in a cell. Mass, momentum and energy are conserved within each cell as well as in the complete computational domain.

One can solve the Navier-Stokes equations exactly by performing Direct Numerical Simulations (DNS). This however introduces a huge demand on the computational grid, and is in practice limited to flows in rather simple geometries at low Reynolds numbers.

There are two main categories of turbulence models available in Fluent: Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulations (LES).

In the former group, equations for the mean flow field are calculated and the effect of turbulence on the mean fields modelled. The instantaneous velocity filed (u_i) can be decomposed into a mean value (U_i) and fluctuating components around the mean ($u_i^{'}$):

$$u_i = U_i + u_i^{'} \tag{2.13}$$

By introducing this decomposition, after some algebra, the RANS equations which describe the mean velocity field are found:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \left(\frac{\partial^2 U_i}{\partial x_j^2} \right) - \frac{\partial}{\partial x_j} \left(\overline{u_i^{'} u_j^{'}} \right) \tag{2.14}$$

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{2.15}$$

where $\nu = \mu/\rho$ is the kinematic viscosity. The term $\overline{u_i^{'} u_j^{'}}$ (the mean of the product of the fluctuating velocity components) is called the Reynolds-stress and must be modelled. There are a number of different RANS models for modelling this term. RANS equations can be rather quick, and are the most commonly used turbulence models in industry.

The latter group filters the turbulent velocity field into large and small structures (eddies):

$$\overline{u_i} = \int G(x, x^{'}) u_i^{'} dx^{'} \tag{2.16}$$

where $G(x, x^{'})$ is a function which is large only when x and $x^{'}$ are far apart. The large eddies are the most energetic and responsible for most of the turbulent transportation and mixing; they are also very much dependent on the flow geometry. Whereas the small eddies are believed to be rather independent of the geometry, and should therefore be simpler to model. The resulting LES equation is:

$$\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j}\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j} \tag{2.17}$$

where $\overline{u_i}$ are the filtered velocity components (large structures), $\overline{p}$ the filtered pressure, and

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \tag{2.18}$$

is the subgrid-scale-tensor, which must be modelled. Hence, LES solves the equations for the large eddies, while the smaller eddies are modelled. Note that although the subgrid-scale-tensor for LES and the Reynolds-stress in RANS play similar roles, the physics they model are different.

LES is in general slower than RANS; the grid requirements are stronger, and LES must be conducted in three dimensions and transient in time while RANS can be conducted in two dimensions and stationary in time. However, turbulent structures which are resolved in LES (up to a point) are not resolved with RANS.

2.2.2 Modelling evaporation

A challenge of using CFD for calculating evaporation and the subsequent transport of vapour is the large separation of scales. Simulating the evaporation from droplets would require computational grid sizes of the order of the droplet size ($\ll 1$ m^2), while the calculations for the subsequent vapour transport may require a computational domain of the order of km. In order to reduce the computational requirements, it is beneficial to have an analytical model for the evaporation rate, and combine this with a CFD calculation of the transport. In this way, the grid requirements can be greatly reduced.

In addition, it is not mandatory to use multi-phase computations with this procedure. Instead the analytical model can be used to produce a source of vapour, and the transport equations for the concentration field can then be solved:

$$\rho\left(\frac{\partial Y_\alpha}{\partial t}+u_j\frac{\partial Y_\alpha}{\partial x_j}\right)=-\frac{\partial J_\alpha}{\partial x_j}+R_\alpha+S_\alpha \tag{2.19}$$

where $Y\alpha$ is the mass fraction of species α, R_α is the production of species α by chemical reactions and S_α is the source term. The diffusion of species α is:

$$J_\alpha=-\left(\rho D_\alpha+\frac{\mu_t}{Sc_t}\right)\Delta Y_\alpha. \tag{2.20}$$

The FFI model is linked to the commercial available CFD software Fluent by use of a so-called User-Defined-Function (UDF). Such UDFs are scripts which is coupled to the Fluent solver. In the present case, UDFs are used both for extracting information from the turbulent velocity field for input to the model and for calculating the evaporation rate; the resulting vapour is introduced to the species transport calculation as a source.

For the UDF for the numerical simulations, u_* is calculated from the solution in each cell at every time step and is thus not constant, and $\mathcal{G}$ and $\mathcal{H}$ are thereby not constant either (as they are functions of u_*). Apart from that, the FFI model is identical "stand-alone" and as included in the UDF.

The default Fluent evaporation model and the two NSWCDD evaporation models are not investigated by numerical simulations in this work, but are instead compared with the analytical model in simple MatLab calculations. The Fluent default and the American hybrid model are potentially grid dependent, as the concentration in the bulk phase in the cells containing the liquid may depend on the size of the cells. The FFI model is not grid dependent.

3 Numerical simulations

Two numerical simulation have been conducted: one Large Eddy Simulation (LES) and one Reynolds Averaged Navier-Stokes (RANS) simulation. The LES simulation is more accurate than RANS and used to study the evaporation model in detail for a short time span, while the RANS simulation is less time-consuming and used to study the time dependence of the analytical evaporation model.

A 2 m long square duct with a cross section of 0.1×0.1 m^2 has been used for the calculations. For the large eddy simulation, there are 200 evenly spread nodes along the streamwise direction (giving a mesh size of 0.01 m), and mesh sizes of 0.001×0.001 m^2 near the wall and 0.003×0.003 m^2 far from the wall in the plane normal to the mean flow direction, resulting in about 2 million cells. For the RANS simulation, there are are mesh size of 0.005×0.005 m^2 in the normal plane, and 0.05 m in the stream wise direction.

3.1 Turbulent velocity field

First the velocity field was calculated. This was done by conducting a periodic simulation in the streamwise direction, where the velocity field at the outlet (at $x = 12$ m) is returned back into the inlet (at $x = 0$ m) (this is in practice an infinitely long duct). A pressure drop of 0.48 Pa/m is imposed in order to get a friction velocity of 0.14 m/s (this is chosen in order to compare the results with experimental measurements [5]). For the LES, a time step size of 0.01 s with a maximum number of 40 iterations per time step was chosen in order to reach numerical convergence. For RANS, a time step of 1 s with 10 iterations per time step were sufficient. The solution were deemed to be converged when the residuals reached numerical convergence, the velocity fields were symmetric, and when the simulated wall friction velocity equals the analytically calculated friction velocity.

For both simulations, 400 velocity profiles at different time step were written to file. These velocity profiles were used to specify the inlet velocity for the evaporation modelling simulations, where periodic boundary conditions could not be used in these cases.

3.2 Evaporation modelling

Liquid mustard agent (HD) particles are introduced into the computational domain by use of the Discrete Phase Model (DPM) of Fluent. A number of identical droplets with volumes of 1 μl ($= 1 \cdot 10^{-9}$ m^3), which corresponds to a mass of $1.279 \cdot 10^{-6}$ kg at a temperature of 188.16 K, are released right above the bottom wall with a velocity component toward the wall. When the droplets hit the wall, they are assumed to stay attached to the wall. On the wall, the particles are given a surface radius of $1.258 \cdot 10^{-3}$ m, corresponding to the initial surface radii from the experiment. Based on the deposited mass, the evaporation rate is calculated and the resulting vapour is given as a source to the species transport model[2].

[2]This might seem a somewhat elaborate method. A vapour concentration calculated from evaporation model by hypothetical droplets without using DPM, could be specified at a wall. However, for coupling the evaporation model with particle transport simulations, in which particles deposited on walls subsequently evaporate, the current method is used.

An important input variable for the evaporation model is the friction velocity, which is read out from the solution. For the LES, the friction velocity is calculated from the velocity gradient in the cell containing the liquid droplet as:

$$u_* = \sqrt{\nu \frac{\partial U}{\partial y}}. \tag{3.1}$$

For the RANS simulation, the friction velocity is calculated directly from the wall shear stress τ_w:

$$u_* = \sqrt{\frac{\tau_w}{A\rho}} \tag{3.2}$$

where A is the cell face area. These are in principle equal, however the former requires very small grid cells in the normal direction near the walls, as the velocity changes quite dramatically in this region. For the RANS simulations, the former method therefore produced erroneous values for the friction velocity.

The transport of vapour throughout the domain is then calculated. The vapour is treated as passive, that is it is assumed that it does not influence the ambient air field. The evaporation model itself is also derived under the assumptions that the vapour can be treated as passive.

Two user-defined-functions are executed. One UDF is executed each time a liquid particle hits a wall in order to attach the particle on the wall. The second UDF is executed at the end of each time step, and calculates the total evaporation rate in each cell that contains droplets. The amount of liquid in each cell are "remembered" by User-Defined-Memory-Inputs (UDMI). One UDMI holds the total amount of liquid in each cell, and another UDMI holds the mass of one droplet in the cell. The number of droplets in a cell can thereby simply be calculated by these.

4 Results

4.1 Results from the numerical simulations

Figure 4.1 shows the normalised evaporation rate calculated with the FFI model for the RANS simulation, compared with the evaporation rate calculated analytically. For the analytical calculation, friction velocities of 0.13 m/s and 0.14 m/s were used. The friction velocity in the numerical simulations were generally in the range of 0.13 to 0.14 m/s. The UDF is in close agreement with the analytical model for a friction velocity of $u_* = 0.13$ m/s. The simulation is conducted to a real evaporation time of 6 hours; if not terminated, the evaporation would continue for another 5-6 hours (as seen from the analytical results).

The evaporation rates in the initial state for the simulations and those calculated analytically are given in table 4.1. The evaporation rates in the two CFD simulations are time-average values over the time interval noted. The analytical evaporation rates are instantaneous values in the early stage of the evaporation process. The two simulations are in good agreement; the cause of the small difference is different values for the friction velocity. The evaporation rates from the simulations are also in good agreement with the analytical results.

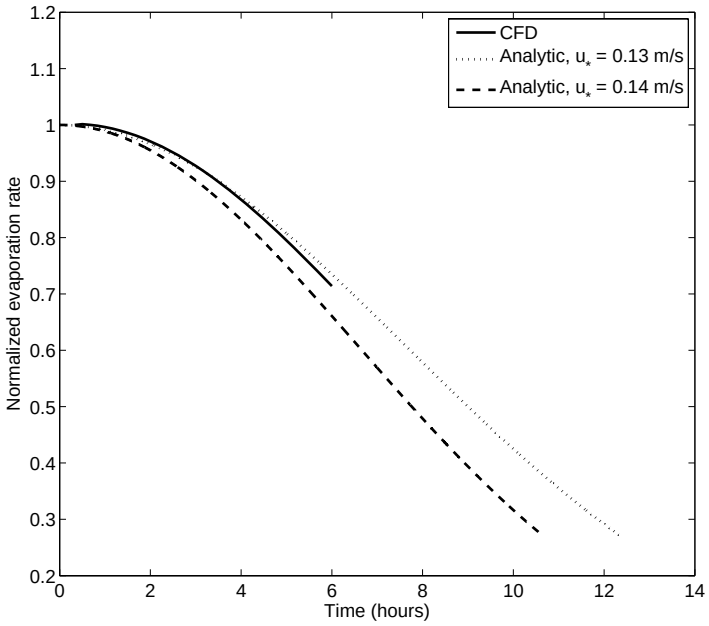

Figure 4.1 Normalised evaporation rate calculated with the UDF for RANS simulations and analytically as function of time.

Method	Evaporation rate (kg/s)
RANS (first 10 min)	$4.321 \cdot 10^{-11}$
LES (4.4 min)	$4.01 \cdot 10^{-11}$
Analytical, $u_* = 0.13$ m/s	$4.12 \cdot 10^{-11}$
Analytical, $u_* = 0.14$ m/s	$4.78 \cdot 10^{-11}$

Table 4.1 The evaporation rates calculated with the CFD simulations and analytically.

The evaporation model included in the UDF is in close agreement with the analytical results, and this gives confidence that the evaporation model can be used for CFD simulations. The model is compared against experimental results and shown to be fairly accurate in a previous report [3].

5 Comparison of the evaporation models

5.1 Comparison with other evaporation models

The FFI model is compared with the two models from NSWCDD described in chapter 2.1.3 and the default Fluent evaporation model described in chapter 2.1.2. By use of the program MatLab, the evaporation rates are calculated for the same scenarios for the various models. In addition the times until all the liquid is evaporated are calculated. The results are also compared against experimental measurements from Navaz *et al.* [5]

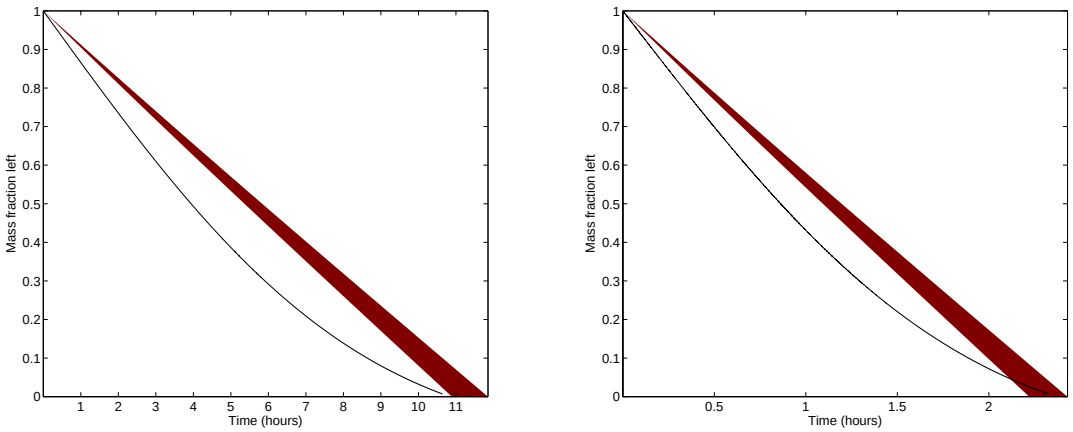

Figure 5.1 Mass fraction left as function of time. The FFI model results are shown as full line. The coloured area is the range given by the ADVEDS model with a slip velocity in the range explained in the text. The figure on the left is for a droplet with volume $V = 1$ μl, temperature $T = 15°C$ and bulk air velocity of $U = 1.77$ m/s, while the figure on the right is for $V = 1$ μl, $T = 35°C$ and $U = 1.77$ m/s.

One difficulty with analytically calculating the evaporation rate with the default Fluent evaporation model and the hybrid model, is determining the concentration in the bulk gas in the cell. This is taken from the numerical simulation (Fluent) ordinarily. For this work, a value for the bulk concentration of $C = 0.14\ C_0$ has been chosen: this is the bulk concentration in the cell containing the liquid droplets as calculated with the Large Eddy Simulation in this work. The value of C has a huge effect on the evaporation rate.

Another uncertainty is the value of the slip velocity, the difference between the velocity of the droplet (which is assumed to be zero) and the ambient wind field. Two values for the wind speed is chosen for the cases with $C = 1.77$ and $U = 3.66$ m/s: the free stream velocity and the velocity at 1 mm from the wall assuming that the so-called log-low is valid in this region. The log-law is not really valid in this region however, a length of 1 mm from the wall corresponds to a length in wall units of about $y^+ \approx 10$, which is in the region between the linear sub-range and the log-law (see for instance [6] for an explanation of near-wall turbulence). For $U = 0.26$ m/s only the free stream velocity is chosen. The evaporation rate is not as strongly dependent on the slip velocity as on the bulk concentration in the cell.

Figure 5.1 shows the remaining mass as function of time calculated with the analytical model and the ADVEDS model. The results from the ADVEDS model are given as the range given by the two values for the slip velocity described above. The models are in good agreement. The ADVEDS model however, gives a near constant evaporation rate throughout the evaporation process, while the analytical model does not.

Table 5.1 shows the total evaporation times calculated with the different models along with the

V (μl)	T (°C)	U (m/s)	τ_{FFI} (hours)	τ_{ADVEDS} (hours)	τ_{Hybrid} (hours)	τ_{Fluent} (hours)	Estimated (hours)
1	15	1.77	10.5	10.5 - 12	10.5 - 12	1.5	9-10
1	15	3.66	6.5	7.5 - 10	8 - 9	1	7-8
1	35	0.26	5.5	6	9	0.5	4-5
1	35	1.77	2.5	2 - 2.5	2	0.2	2
6	15	1.77	19.5	19.5 - 24.5	21 - 24	3.5	20-24
6	35	0.26	10	11	18	1	14-15
6	35	1.77	4	4 - 4.5	4 - 4.5	0.5	4.5-5
9	35	1.77	5	4.5 - 5	4.5 - 5	0.7 - 0.8	4

Table 5.1 Total evaporation times calculated with the various models and estimated from the experimental data [5] as a function of friction velocity and free-stream temperature.

evaporation times estimated from the experiments. For the Fluent default model, the evaporation time is estimated from the initial evaporation rate. In reality, the height of the droplet, which is included in the model, decreases in time, thus leading to a decrease of the evaporation rate in time, and the estimated time given is therefore a minimum value.

The FFI model, the hybrid and the ADVEDS model are in very good agreement. The Fluent default model, however, gives about an order of magnitude shorter evaporation than the others. It should be mentioned however, that the value used for the bulk concentration is taken from a simulation with the FFI model, and the "true" value for the default model is not easy to determine analytically. It should really be calculated in a numerical simulation with this evaporation model. It is worth mentioning that the disagreement between the default Fluent model and the others are quite constant for all the data sets. In fact, the results from the Fluent default model is in agreement with the other models if a value for the bulk concentration of $C = 0.9C_0$ is chosen; however, *a priori* it is unclear why this value should be correct.

6 Concluding remarks

An analytical evaporation model, developed at FFI [3], has been integrated in CFD software and the integration has been verified. The model is dependent on the friction velocity, which is read out from the solution. The evaporation rate from a number of droplets or a small pool is calculated, the resulting vapour is introduced into the computational domain, and the transport of vapour simulated. The model is tested with the CFD software Fluent, and gives results in close agreement with the analytically calculated evaporation rate. The model is compared with other evaporation models, and shown to be in fairly good agreement with two models from NSWCDD. By comparing against experimental measurements it is evident that both the FFI model and the NSWCDD models constitute a substantial improvement to the default Fluent evaporation model.

A positive property with the analytical model, is that it is grid independent. It can also just as easily

be used both analytically and with CFD software. Other evaporation models for CFD calculations however, like the default Fluent model and the hybrid model, are grid dependent; the value for the bulk concentration is dependent on the cell sizes. These two models also include parameters read out from the solution, for which reliable values may be difficult to obtain analytically.

The model can easily be introduced into other numerical software also, including faster dispersion models and hazard prediction and assessment tools.

There are plans to develop the evaporation model further (see [3]). The User-Defined-Function, which couples the model to CFD calculations, will be updated accordingly.

References

[1] Thor Gjesdal. Oversikt over modeller for spredningsberegning (an overview of models for dispersion modelling). *FFI/NOTAT-2003/00581*, 2003. Norwegian Defence Research Establishment (In Norwegian).

[2] NATO/RTO/SAS-061. Defence against CBRN-attacks in a changing NATO strategic environment. *NATO/Research and Technology Organization (RTO)/System Analysis and Studies (SAS)-061 Technical Report*, 2009. "RESTRICTED".

[3] Thomas Vik and Bjørn Anders Pettersson Reif. Modeling the evaporation from a thin liquid surface beneath a turbulent boundary layer. *FFI/RAPPORT-2010/00254*, 2010. Norwegian Defence Research Establishment.

[4] G Desoutter, C Habchi, B Cuenot, and T Poinsot. Dns and modeling of the turbulent boundary layer over an evaporating liquid film. *Int. J. Heat and Mass Transf.*, pages 6028–6041, 2009.

[5] H K Navaz, E Chan, and B Markicevic. Convective evaporation model of sessile droplets in a turbulent flow - comparison with wind tunnel data. *Int. J. Thermal Sciences*, 47:963–971, 2008.

[6] Stephen B Pope. *Turbulent flows*. Cambridge University press, 2000.