Simulation of transport, evaporation, and combustion of liquids in large-scale fire incidents

Topi Sikanen
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A doctoral dissertation completed for the degree of Doctor of Science (Technology) to be defended, with the permission of the Aalto University School of Engineering, at a public examination held at the lecture hall R1 (Rakentajaukio 4 A, Espoo) of the school on 19th January 2018 at 12:00.

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Abstract

Combustible liquids are often present in large quantities in industrial facilities and in transportation. Leaks, vessel ruptures, transportation accidents and terrorist attacks involving liquids may lead to large scale fire incidents. Analyses of such incidents are needed in the safety analyses of nuclear power plants and other critical infrastructure. However, large scale incidents may be outside the area of validity of empirical models. Development and validation of numerical simulation methods are therefore needed.

This thesis has two objectives. The first is to develop and validate spray boundary conditions that can be used to model spray injection of water mist systems or for modeling liquid dispersal. The second is to predict burning rates of liquid pool fires starting from first principles. Large eddy simulation is used for the Eulerian gas phase solution and Lagrangian particle tracking for the sprays.

The spray model is developed and validated using data from experiments on high-pressure water mist nozzles and liquid-filled missile impacts. Suitable droplet size distributions and initial velocities for use in spray simulations are determined from experimental data. The spray structure and entrainment into the sprays are predicted with reasonable accuracy. The conclusion is that liquid dispersal from missile impacts can be simulated using the same spray models as for water mist sprays.

The burning rate of the liquid pool is calculated on the basis of vapor pressure and a mass transfer calculation at the liquid surface. One dimensional heat transfer by conduction and radiation within the liquid is considered. Effective absorption coefficients are determined for use with a one-dimensional radiation transport equation. An enhanced thermal conductivity model accounts for in-depth convective heat transfer. The conclusion is that inclusion of spectrally resolved radiation calculations and of lateral convection may be necessary for predicting the temporal development of the burning rate.

Finally, the models are applied to the full-scale simulation of an airplane impact on a nuclear island. The predicted fireball lifetimes and sizes compare favorably with available empirical correlations. A significant amount of the fuel involved accumulates on the surfaces around the impact point.

Keywords fireball, pool fire, spray, plane crash

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Tekijä
Topi Sikanen

Väitöskirjan nimi
Nesteiden kuljettumisen, haihtumisen ja palamisen simulointi suurissa onnettomuksissa

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Tiivistelmä

Tällä oppioppetöyjällä on kaksi tavoitetta. Ensimmäinen tavoite on kehittää ja validoida vesisuhkureunaehoto, jota voidaan käyttää vesisumujärjestelmien simuloinnissa tai nesteiden levimisen mallintamiseen. Toinen tavoite on ennustaa nestealtaita palamisnopeudelementen lähtien fyysiallista perusteesta. Kaasufaasin simuloinnissa käytetään suurten pyörteiden menetelmää (LES) ja siperoiden simuloimati LE (Lagrangian-Eulerian) -menetelmä.


Kehtettyjä malleja sovelletaan ydinvoimalaitokseen kohdistuvan lentokonetörmäyksen simulointiin. Ennustetut tulipallon kestoja ja halkaisijat vastaavat melko hyvin empirisiä malleja. Merkittävä määrä poltoainetta kertyy törmäyspiisteen ympärillä oleville pinnoille.
Preface

The work in this thesis was carried out at VTT Technical research center of Finland between 2010 and 2017. Parts of this work were also carried out at the National Institute of Standards and technology in Gaithersburg, MD, USA.

My career as a Fire Scientist began when I applied for a Master's thesis position at VTT. Initially, the subject was going to be statistical, i.e. risk analysis of forest fire smoke or something to that effect (I forget). However, on my first day, the subject had changed, and I was asked if I wanted to develop a model for firebrands in FDS. I thought to myself “How hard can it be?”. This illustrates very well how little I knew of fluid dynamics or of Fire.

My ten years at VTT have certainly been a learning experience. Each project and paper seems to lead to new questions and problems. Perhaps one of the most important lessons has been that papers do not need to (and seldom do) solve all of the world's problems. Instead, they are a description of work done up to that point.

I thank Simo Hostikka for agreeing to be the supervisor and instructor for this thesis in 2013. Serious progress on the thesis began under his supervision. I also thank Esko Mikkola, who was my master's thesis instructor and initially also agreed to be the instructor for my PhD thesis. I am sincerely grateful to the pre-examiners for their valuable comments.

Thank you to people at Kemistintie 3 for the great work ambiance, and for making it an easy and pleasant place to work. A very special thank you goes to the “fire people” still left at VTT: Anna, Tuula, Antti, Terhi, Timo and Jukka. I am grateful to our team leader Eila Lehmus for her encouragement and for arranging financial support for the finalization of this thesis. I am also grateful to Dr. Kevin McGrattan for the opportunity to spend a year as a guest researcher at the National Institute of Standards in Gaithersburg, MD.

I thank the IRSN for providing the experimental data for our use. Special thanks go to Pascal Boulet (Université de Lorraine) for arranging the measurements of the spectral absorption data used in Paper IV.

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List of publications

This thesis is based on the following original publications which are referred to in the text as I–V. The publications are reproduced with kind permission from the publishers.


Author’s contributions

Publication I: “Modeling and simulation of high pressure water mist systems.”

The author wrote the paper and was responsible for the modeling and simulation of the experiments. The author also developed the spray boundary condition used for spray simulations. Co-authors were responsible for conducting the experiments and gave comments and feedback on the manuscript.

Publication II: “Experimental characterisation of sprays resulting from impacts of liquid-containing projectiles.”

The author only analyzed the droplet distributions resulting from impacts of liquid filled missiles and participated in the writing of the article. Markus Honkanen conducted the direct imaging measurements of droplet size. Ari Vepsä was responsible for conducting the missile impact experiments. Ari Silde analyzed the spray front propagation. Simo Hostikka was the lead author of the paper.

Publication III: “Numerical Simulations of Liquid Spreading and Fires.”

The author was responsible for writing the paper and performed all the simulations. Co-author developed the model of the nuclear island and gave comments and feedback on the manuscript.

Publication IV: “Modeling and simulation of liquid pool fires with in-depth radiation absorption and heat transfer.”

The author was responsible for writing the paper and performed the modeling and simulation. The author also developed the methods for determining effective absorption coefficients and effective thermal conductivities. Co-author gave comments and feedback on the manuscript.

Publication V: “Predicting the Heat Release Rates of Liquid Pool Fires in Mechanically Ventilated compartments.”

The author was responsible for writing the paper and designed and conducted the simulations. Co-author gave comments and feedback on the manuscript.
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Publications I–V
List of symbols

\( \alpha \)  
Droplet volume fraction (-)

\( c \)  
Total molar concentration (mol/m³)

\( C \)  
Empirical coefficient (-)

\( c_p \)  
Specific heat capacity (kJ/kg K)

\( D \)  
Diffusion coefficient (m²/s)

\( d \)  
Droplet diameter (m)

\( g \)  
gravitational acceleration vector

\( h \)  
Sensible enthalpy (kJ/kg)

\( h_m \)  
Mass transfer coefficient (m/s)

\( \Delta h_v \)  
Latent heat of evaporation (kJ/kg)

\( \Delta h_g \)  
\( \Delta h_v + \int_{T_0}^{T} c_p(T)dT \). Total heat of evaporation (kJ/kg)

\( I \)  
Intensity (W/Sr·m²)

\( k \)  
Thermal conductivity (W/ m² K)

\( \kappa \)  
Absorption coefficient (1/m)

\( \mu \)  
Dynamic viscosity (Pa·s)

\( \nu \)  
Kinematic viscosity (m²/s)

\( \rho \)  
Density (kg/m³)

\( R \)  
Universal gas constant \( R = 8.3144598 \) (kg m² s⁻² K mol⁻¹)

or droplet radius (m)

\( \tau \)  
Stress tensor
\( \tau \) Characteristic time (s)

\( T \) Temperature (K)

\( u \) Velocity (m/s)

\( V \) Particle velocity (m/s)

\( p \) Pressure (Pa)

\( J \) Mass flux tensor

\( L \) Characteristic length (m)

\( M \) Mass (kg)

\( N \) Number of moles (mol)

\( \dot{q}'' \) Heat flux vector

\( Y \) Mass fraction (kg/kg)

\( X \) Volume fraction (mol/mol)

\( \langle \cdot \rangle \) Expected value

\( \langle x \mid y \rangle \) Expected value of \( x \) conditional on \( y \)

\( \|x\| \) Vector norm \( \|x\| = \sqrt{\sum_{i} x_i^2} \).

**Superscripts**

\((i)\) \( i \)-th particle property

\( S \) Property evaluated at a surface

\( \infty \) Property evaluated in “free stream” or ambient conditions

\( @p \) Property evaluated at particle position

\( '' \) Flux \((-/m^2)\)

\( ''' \) Volumetric term \((-/m^3)\)

\( . \) Rate \((-/s)\)

**Subscripts**

\( \alpha \) Species \( \alpha \)

\( b \) Boiling temperature or blackbody intensity

\( f \) Fuel
<table>
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<td>$g$</td>
<td>Gas phase property</td>
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<tr>
<td>$l$</td>
<td>Liquid phase property</td>
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<tr>
<td>$\lambda$</td>
<td>At wavelength $\lambda$</td>
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<tr>
<td>$o$</td>
<td>Oxidizer</td>
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<td>$t$</td>
<td>Turbulent</td>
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<tr>
<td>$r$</td>
<td>Radiant</td>
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1. Introduction

1.1 Motivation and background

Liquid fuel spills present a potential fire hazard in many situations. The fuel dispersal leading to the formation of the spill may be a result of e.g. a pipe burst, vessel rupture, transport accidents, arson or terrorist attacks. Depending on the dispersal process, these incidents may lead to fireballs, pool fires, or spill fires. Evaluation of the consequences of such incidents is needed in the safety analyses of critical infrastructure.

The most important parameter in determining the impact of a fire on its surroundings is the heat release rate (HRR). The heat release rates of spill fires and pool fires are known to depend on the pool size. The pool size, in turn, depends on the fuel dispersal process. Spill fire sizes and heat release rates have been studied extensively. However, the conditions involved in the incident, such as the geometry, wind and oxygen concentration, as well as the fuel dispersal process, may be outside the domain of validity of traditional empirical methods.

For example, aircraft impacts must be considered in safety analyses of nuclear power plants (NPPs) [1]. Initially, the impact was envisioned to be from a small aircraft or possibly a fighter plane. Following the September 11 terrorist attacks in 2001, these analyses have been extended to assume the impact of a large commercial aircraft [2].

Such an aircraft can damage safety-related structures and components through mechanical impact and fire. Fires induced by an airplane impact may influence the NPP by three different mechanisms. Initially, a large fireball is created by the fuel cloud erupting from the breaking fuel tanks. This fireball has a duration of a few seconds and can be a hundred meters in diameter [3]. The most serious threat from a fireball to its surroundings is thermal radiation. The dose of thermal radiation received by a target is dependent on the size and duration of the fireball.

Only a fraction of the fuel carried by the plane will burn in the initial fireball [4]. The remaining part of the fuel will accumulate and burn in pools near the aircraft impact position. The size and burning rate of the pool fire depend on the geometry, properties of the roof and ground surfaces, and possible fire suppression activities.

The third mechanism involves the penetration of aviation fuel inside the plant through openings. These openings may exist beforehand (e.g. for ventilation) or be
created by the aircraft impact. Even if the amount of penetrated fuel is small, it can cause a rapid ignition of existing fire loads and result in internal fires.

Each portion of the problem touches on a widely researched problem in fire safety science: pool fires, fireballs and spray flames. However, the conditions are well outside the region of validity of most correlations. Because of this, their analysis would require the use of simulation software.

Fire safety analyses are commonly carried out using computational fluid dynamics (CFD) software. Although CFD models could in theory be used to predict the HRR of fires, this is usually predicted using correlations. The capability of CFD models hinges on their ability to predict the important phenomena such as radiative heat transfer to the surface, fuel dispersion and suppression activities.

The methods developed in this thesis can be applied in more general settings than just nuclear safety. For example, pool fires are a significant fire hazard in all industries, not just the nuclear industry, and not only after a plane crash. Fireballs, on the other hand, can be formed from ruptures of pressure vessels or pipelines. Water mist is, of course, a widely used method of fire suppression.

The issues faced when modeling the sprays from liquid-filled missiles and water mist systems are the same. The first problem is characterization of the initial spray in terms of droplet sizes, velocities, and shape. The second problem is the simulation of spray transport. Correct prediction of the two-way coupling between the gas phase and the spray is crucial for successful simulations of either phase. From the computational standpoint, the simulation of high-pressure water mist systems and the simulation of liquid dispersal from missile impacts are both high-speed simulations. The droplet sizes are similar in both cases, and even the droplet velocities are of the same magnitude.

1.2 Objectives and scope of the thesis

The purpose of this thesis is to develop numerical models for the transport, evaporation, and combustion of liquids present in large-scale fire incidents. The modeling efforts are limited to developing the sub models and boundary conditions for an existing CFD code Fire Dynamics Simulator (FDS), and to demonstrating their applications for fire safety problems. Each paper of this thesis aims to improve one aspect of the modeling.

The objectives of Paper I are

1. the development of a spray boundary condition for use in high-pressure water mist simulations,
2. validation of the spray model in FDS for simulations of high-speed liquid sprays, and
3. modeling dense spray effects in an LES context.

The objectives of Paper II are (the contribution of the author)

1. characterization of the initial spray from impacts of liquid-filled missiles.
The objective of Paper III is to "develop and validate a computational fluid dynamics (CFD) methodology for predicting the spreading and combustion of liquid fuel released upon an aircraft impact." This overall objective is broken down into smaller goals:

1. development and validation of the spray boundary condition describing the fuel release.
2. validation of FDS predictions of fireball diameters and lifetimes.
3. investigation of the amount of liquid fuel left unburnt in the initial fireball following a crash
4. evaluation of the adequacy of physical separation based on a full-scale simulation study of aircraft impact on a nuclear island.

The objectives of Paper IV are

1. prediction of the liquid surface evaporation rate using a boundary condition based on an engineering mass transfer expression,
2. development of an appropriate technique for the specification of the liquid phase radiation absorption coefficients,
3. investigation of the importance of in-depth heat transfer in laboratory scale (0.5-3 meters) pool fires, and
4. validation of the proposed modeling approach using experimental results for different fuels.

The objectives of Paper V are

1. validation of the modeling methodology proposed in Paper II for the simulations of pool fires in mechanically ventilated compartments, and
2. further investigation of the in-depth heat transfer effects on the development of liquid pool fire burning rates.

Figure 1.1 visualizes the goals and contributions of this thesis.
Figure 1.1 Hierarchical chart illustrating the overall goal and contribution of this thesis. The Roman numerals in parentheses (I-V) indicate the paper in which the issue is discussed. The marking (S) indicates that additional work is described in this thesis summary.

1.3 Outline

The main text of this thesis summary is organized as follows.

Section 2 presents a literature review of fire modeling in general, and of modeling of pool fires and liquid sprays in particular.
Section 3 describes the models used and developed in Papers I-V. The first part of the section presents an overview of the governing equations of the CFD software. The rest of the section describes the methods developed in Papers I-V.

Section 4 divides the results of the research into spray modeling, liquid pool fire modeling, and risk analysis. The sections on spray and pool fire modeling further divide the results into verification and validation. Papers I-V describe the Validation work. This thesis summary adds a description of the verification work.

Section 5 summarizes the conclusions from the research.
Section 6 presents suggestions for future research topics.
2. Literature review

2.1 Governing equations

2.1.1 Governing equations for the gas phase

The governing equations of compressible viscous follow from the conservation of mass, momentum, species, and enthalpy. The mass conservation equation is

\[ \frac{\partial \rho}{\partial t} = \dot{m} \tag{1} \]

where \( \rho \) is the density, \( \dot{m} \) is the mass source term due to e.g. evaporation, and \( \frac{\partial \phi}{\partial t} = \frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\phi \) is the substantial derivative. The conservation of momentum can be written as

\[ \frac{\partial \rho \mathbf{u}}{\partial t} = \rho \mathbf{g} - \nabla p + \nabla \cdot \mathbf{t} + \mathbf{f} \tag{2} \]

In the momentum equation, the body force term \( \mathbf{f} \) accounts for external forces acting on the fluid. Conservation of species is written as

\[ \frac{\partial \rho Y_\alpha}{\partial t} = \nabla \cdot \mathbf{j}_\alpha \tag{3} \]

where \( Y_\alpha \) is the mass fraction of species \( \alpha \). The species mass flux \( \mathbf{j}_\alpha \) accounts for the diffusion mass flux. Finally a conservation equation for the sensible enthalpy \( h \) is given by:

\[ \frac{\partial \rho h}{\partial t} = \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{q}^* \tag{4} \]

The heat flux vector \( \mathbf{q}^* \) includes heat transport by conduction and radiation. The system of equations (1)-(4) is closed by the equation of state. For most fire situations, the ideal gas equation of state is sufficient.

\[ p = \frac{\rho RT}{W} \quad W = \frac{1}{\sum \omega \gamma_\alpha / \mathcal{W}_\alpha} \tag{5} \]

With a different choice for the equation of state, equations (1)-(4) are equally valid for describing the motion of liquids.

2.1.2 Radiation

Radiation transport is usually the dominant heat transfer mechanism in fires. In a non-scattering medium, the radiation transport equation (RTE) in direction \( s \) is given by

\[ s \cdot \nabla I_s = \kappa_s I_s + \kappa_s I_{s,b,s} \tag{6} \]

\(^1\) This equation may also be written in terms of temperature, enthalpy, energy or sensible energy (see e.g. [130]).
Here, $\kappa$, $I_{b,\lambda}$, and $I_\lambda$ are the absorption coefficient, black body intensity and intensity at the wavelength $\lambda$. The radiation transport gives rise to a source term in the energy equation:

$$-\nabla \cdot \dot{q}^e_r = \int_0^\infty \kappa \left[ U - 4\pi I_{b,\lambda}(x) \right] d\lambda \; ; \; U = \int_{4\pi} I_\lambda(x, s') ds'. \tag{7}$$

From a numerical standpoint, the above equation is problematical. Equation (7) involves a double integral: one over the solid angle and another over all the wavelengths. In most fire applications, the gray gas assumption is invoked, removing the wavelength dependence.

### 2.1.3 Governing equations of dispersed phase

Equations governing the motion of a single particle are quite well known by now. Several books [5–7] and review articles [8–10] have been written on the subject. Maxey and Riley [11] derived an expression for the forces acting on a rigid spherical particle in non-uniform flow

$$\frac{d m \nu}{d t} = F_D + F_G + F_P + F_H + F_L. \tag{8}$$

On the LHS, $m$ and $\nu$ are the mass and the velocity of the particle. The force terms appearing on the RHS are the drag force, gravitational acceleration, pressure gradient force, the Basset history force and lift force. The linear decomposition of forces in Eq. (8) is not always valid, since there may be non-linear interactions between the forces. These interactions are poorly understood and are usually neglected [8]. The last three terms are generally found to be negligible when the density of the particles is much higher than that of the carrier phase [8,9,12]. This type of model is commonly called a “quasi-steady drag” model since the unsteady terms are ignored.

If the droplet does not affect the carrier phase, the model is described as one-way coupled. In sprays, the influence of the droplets on the carrier phase usually needs to be taken into account. Typically, Lagrangian particle models only consider two-way coupling of the gas phase and the dispersed phase. The two-way coupling means that each particle interacts with the carrier fluid individually. Momentum lost from a particle is gained by the fluid and vice versa.

If the spray is dense enough, the droplets may start to travel in each other's wakes. The Lagrangian-Eulerian model cannot capture these effects for two reasons: First, the Lagrangian particles have no volume in the Eulerian space, preventing the model from seeing effects that take place in the length scale of the droplet diameter. Secondly, the effects of this length scale would be sub-grid scale in most practical simulations. Therefore, these effects need to be modeled. This kind of modeling is sometimes called three-way coupling.

These aerodynamic interactions are often assumed to become important when the average droplet spacing is less than ten droplet diameters [8]. Ten droplet spacings correspond approximately to a droplet volume fraction $\alpha = 0.01$. Volume fractions as high as this can sometimes be achieved inside the sprays considered.
in this thesis. If the spray was even more dense, particle-particle collisions or four-way coupling would need to be considered.

2.1.4 Governing equations for liquid evaporation

Equations (1)-(4), with the appropriate equation of state, describe the motion of both gases and liquids. At the interfaces of liquids and gases, such as on the surface of a liquid droplet or on the surface of a liquid pool, models are needed for the interfacial fluxes. This section discusses evaporation mostly from the perspective of pool fires. The discussion in this section is equally valid for evaporation from liquid droplets. In practice, droplets are usually much smaller than the computational grid, leading to somewhat different models of evaporation.

In a binary mixture of gases A and B, the molar flux of A relative to species B, in the z-coordinate direction, is [13]

\[
\dot{N}_A^s = c D_{A,B} \frac{\partial X_A}{\partial z} + X_A (\dot{N}_A^s + \dot{N}_B^s).
\]

Here \( D_{A,B} \) is the binary diffusion coefficient of A in B, \( X \) is the volume fraction of a species, and \( c \) is the total molar concentration. In the case of evaporation from a surface, we can take species A to be our evaporating species and B to be air. We will furthermore assume that the molar flux of air at the evaporating surface is zero, \( \dot{N}_B^s = 0 \). The evaporated molar flux from the surface can then be calculated from

\[
\dot{N}_A^s = c \frac{1}{1 - \gamma_F} \delta_F \left( \frac{\partial X_A}{\partial n} \right)^s = c u_S.
\]

Here \( u_S \) is the Stefan velocity, the velocity caused by the evaporation, \( \delta_F \) is the binary diffusion coefficient of the evaporating species in the ambient air, and \( n \) denotes surface normal direction. Terms marked with the superscript \( s \) are evaluated at the surface.

For an ideal gas the volume fraction can be calculated from the Clausius-Clapeyron relation for the partial pressure of saturated vapor:

\[
X_A = \frac{p_{sat}(T)}{p_b} = \exp \left[ -\frac{\Delta h}{R} \left( \frac{1}{T} - \frac{1}{T_b} \right) \right].
\]

On the liquid side, full Navier-Stokes equations would be needed to capture all the physics involved in predicting the surface temperature \( T^s \). In numerical simulations, one of the main difficulties involved in the solution of Equation (10) is evaluation of the vapor volume fraction gradient \( (\partial X_F/\partial z)^s \). The length scales involved become very small as the surface is approached. In order to resolve the concentration boundary layer, increasingly fine grids are needed.

In numerical simulations, the near wall grid resolution is often reported in terms of non-dimensional distance \( y^+ \). This is the distance from the surface to the first grid cell center divided by the local viscous length scale, \( \delta_\nu \) [14]:

\[
y^+ = \frac{1}{2} \frac{\delta n}{\delta_\nu}; \quad \delta_\nu = \frac{\mu}{\rho u_\tau}; \quad u_\tau = \sqrt{\tau_w/\rho}.
\]

17
Here $\tau_w = \mu \partial |u|/\partial n$ is the viscous stress evaluated at the wall, and $u_*$ is the friction velocity. For a direct evaluation of the volume fraction gradient, a near wall grid resolution of $y^+ = 1$ is needed. Such grid resolutions are often infeasible. Therefore, the near wall gradients need to be modeled.

A commonly used approximation is based on the "film theory" (See, e.g. [13, pp 554-580]). If we assume that the vapor mass flux is constant within a thin film near the boundary, Equation (10) may be integrated over the film thickness $\delta$ to give

$$N^* = c \frac{D_F}{\delta} \log \left( \frac{1-x_f^\infty}{1-x_f^s} \right).$$

(13)

Here $X_f^\infty$ is the "free stream" volume fraction of the evaporating species.

In the literature on spray evaporation Equation (13) is often written in terms of mass fractions instead of volume fractions. The difference between formulations based on molar fractions and mass fractions is in the assumptions needed for integrating Eq. 9. When molar fractions are used the assumption is that the total molar concentration and diffusivity stay constant. This is true in isothermal systems with constant pressure. If mass fractions are used, the total density of the gas mixture is held constant. Neither of these assumptions can be rigorously defended, but the former assumptions are perhaps slightly less restrictive.

Equation (13) still requires an estimate for the film thickness $\delta$. This can be done e.g. by relating the film thickness to a mass transfer coefficient:

$$\frac{D_F}{\delta} = \frac{ShD_u}{L} = h_m.$$

(14)

In the above, $Sh$ is the Sherwood number, $h_m$ is the mass transfer coefficient, and $L$ is the characteristic length. Models based on film theory are commonly used to predict droplet evaporation (See, e.g. [7, pp. 9-29]). Droplets are usually much smaller than the grid size in CFD codes, and the "free stream" values and the length scale $L$ have natural definitions. This is not the case when Eq. (13) is applied as a wall model in CFD.

In wall-bounded flows, a commonly used method for approximating the wall normal gradients is to use mixing length arguments to derive an analytical profile for the scalar near the wall. In the traditional flat plate boundary layer theory, this gives rise to the log-law velocity and scalar profiles. One problem with using the log-law for evaporation problems is the non-zero wall normal velocity or "blowing." Blowing changes the shapes of the near wall velocity and concentration profiles. The overall effect of blowing is to decrease the convective heat flux to the wall and to reduce the wall shear stress. [15, pp. 414-493]

Desoutter et al. [16] attempted to derive wall models that would account for the effect of blowing. They performed DNS simulations of the boundary layer above an evaporating liquid film in turbulent channel flow. By introducing new scaling for the variables, they were able to recover the traditional log law behavior of the boundary layer in the presence of evaporation. However, the parameters of their wall-law were found to be case dependent, reducing the usefulness of the approach.

Perhaps due to the above-described difficulties in wall modeling, many pool fire models ignore the boundary layer resistance to mass transfer (e.g. [17,18]). Instead,
they assume that the amount evaporated is ultimately determined by the energy balance at the surface [18]

\[ \dot{m}^* = \frac{\dot{q}_{net}^*}{\Delta h_g} \]  

(15)

The exact way in which \( \dot{q}_{net}^* \) is calculated varies from author to author. In the context of pool fire modeling, this approach can be justified by examining equation (10). The volume fraction of the evaporated species \( X_A \) grows as the surface temperature approaches boiling point. Consequently, the denominator in equation (10) tends towards zero and the mass flux grows without bound. When the surface temperature is near the boiling point, evaporation mass flux is limited only by the amount of incoming heat flux. However, blowing tends to decrease the incident convective heat flux and this effect may be important if convection heat transfer is the dominant mode of heat transfer.

2.2 Spray characterization

2.2.1 Structure and breakup of sprays

Liquid sprays are used in many industrial processes, including combustion, coating and fire suppression to name just a few. Regardless of the particular application, the efficiency of the system depends on the properties of the spray. For purposes of numerical simulations, the important properties of the sprays are the initial droplet velocity and size distribution.

The processes that lead to formation of a spray from a continuous jet or sheet of liquid are called atomization or breakup processes. Figure 2.1 shows a close-up picture of the spray atomization processes in a Spraying Systems LN-02 water mist nozzle. Spray formation is often broken down into two steps. The first step is the primary atomization. Typically, primary atomization is achieved by injecting a jet or sheet of liquid into a gas. The shear between the gas and the injected liquid causes instabilities to form on the liquid surface. These instabilities grow until the continuous liquid is broken into fragments [19]. The fragments produced by the primary atomization are often relatively large and may be deformed by the aerodynamic forces acting on them. If the deformation is sufficient, the fragments may become unstable and break up into smaller pieces. This process is called secondary breakup [20]. The breakup of the droplets continues as long as the aerodynamic forces are strong enough to overcome the surface tension forces holding the droplet together. The balance between surface tension and inertia is usually reported in terms of

\[ We = \frac{\rho V^2 d}{\sigma} \]  

(16)

where \( V \) is the velocity of the fragment (or droplet), \( d \) is the diameter of the droplet and \( \sigma \) is the surface tension. The critical Weber number at which breakup processes begin is between 10 and 20 [7, p.144].
The breakup of water jets has been a subject of active research for many years, and the results of the research have been presented in many reviews on the subject [20–22].

From a practical standpoint, the structure of a spray resulting from the primary and secondary atomization depends on several factors. First is the existence of disturbances in the initial liquid flow. Second is the liquid surface tension. Due to differences in surface tension, different fluids may produce different sized droplets, even if they are generated by the same nozzle.

Simulation of all the primary and secondary atomization is usually not feasible. Sometimes a stochastic model is used to account for the entire spray formation process [23–26]. In other cases the breakup processes may be modeled by deterministic models, with the stochastic component stemming from the droplet motion. The modeling of spray atomization is still an active research topic.

![Image of a Spraying Systems LN-02 water mist spray](image)

**Figure 2.1** Close-up image of a Spraying Systems LN-02 water mist spray, showing primary and secondary atomization processes occurring. Picture from the Tampere University of Technology.

### 2.2.2 Water mist sprays

Commercially available sprinklers may differ substantially in the spray pattern they produce as well as in droplet sizes and velocities of the sprays. Water mist is a particular type of fire suppression spray that is characterized by small droplet size (99% of the spray volume is composed of droplets that are under 1000 microns in diameter [27]).

The usual way of characterizing sprinkler sprays is by measuring spray dispersion patterns. The dispersion patterns are measured by placing collection bins on the floor and measuring the water flux into each bin. Sprinklers are usually designed with a certain shape of dispersion pattern in mind. This kind of data is not useful for the development of spray models for use in CFD. Experimental
uncertainties and low resolution also diminish the usefulness of the data for validation purposes.

Measurements in the near field of the spray are needed for use in simulations. This has been recognized in the research community, and progress has been made in the detailed characterization of fire sprinkler sprays [28,29]. However, these efforts have mostly focused on traditional sprinkler sprays and not on water mists. Detailed measurements of water mist sprays have been conducted with PDPA and using direct imaging techniques [30–34]. Since water mist is often produced by pressure-swirl type nozzles, a significant amount of research is available on the spray structure and droplet size in the context of combustion applications.

2.2.3 Sprays from liquid-filled missile impacts

In addition to spray nozzles, the spray may be a result of a transportation accident or a tank rupture. From the perspective of this thesis, the most important class of transportation accidents is aircraft impacts. In a plane crash, the fuel dispersal process is similar to the spray formation process in a pressure-atomized spray. Tieszen [35] summarized the process as follows: First, due to the rapid deceleration of the crashing plane, liquid fuel is ejected from the tanks through ruptures formed because of the crash. What follows is the primary breakup phase, in which the discharged liquid sheets undergo atomization due to the instabilities generated by aerodynamic drag. The resulting liquid fragments are usually so large that the aerodynamic forces deform them. The deformation increases until the fragment breaks up into smaller droplets.

Unlike the spray formation from a nozzle, the spray formation from a liquid tank impact is not very well characterized. The ejection velocity of the liquid is unknown, and the size and shape of the initial liquid sheets are uncertain. Fragments of the impacting structure may also interfere with the spray.

Experimental data on the sprays formed by aircraft impact are scarce. The focus of experimental research has usually been on either crash worthiness of tanks (castor tanks or fuel tanks) or the effect of the impact on structures. Sandia National Laboratories conducted a full-scale test, in which a Phantom F-4 aircraft carrying 4.8 tons of water impacted a reinforced concrete target [36–38]. They did not make detailed measurements of water dispersal, but video footage shows the propagation of the spray cloud (See Figure 2.2). However, at least part of the cloud seen in the footage is made up of dust particles and debris of the impacting plane.
VTT conducted a series of experiments with liquid-filled missiles impacting on a concrete block. Droplet size distributions were measured using a direct imaging method, and the resulting spray shapes were recorded on high-speed video. The results of the spray characterization experiments are reported in a paper by Slade et al. [39] and in Paper II.

Very few attempts at predicting the liquid dispersal process are available in the open literature. Brown et al. [40,41] coupled a transient dynamics code Presto with a low-Mach number fire code Fuego to predict the liquid dispersion from the high-speed impact tests of Jepsen [42]. They used Smoothed Particle Hydrodynamics (SPH) to predict the motion of liquid within the tank on impact. The particles from the SPH solution were then transferred to the fire code once the distance between the particles dropped below a certain threshold level. They found that their model was able to reproduce the observed liquid dispersal patterns reasonably well. Brown et al. did not compare the droplet size predictions with experimental results [41].

Figure 2.2 Still images from the video clips of the Phantom F-4 test by Sandia National Laboratories

Figure 2.3 Spray front in the IMPACT experiments.
2.3 Modeling liquid pool fires

2.3.1 Physical mechanisms

Pool fires have been studied for decades, and the results have been collected in several review articles [43–46]. The result of such studies has usually been an empirical or semi-empirical correlation for the steady state burning rate of a pool fire as a function of the pool size. A recent example is a study by Ditch et al. [47], in which the authors correlated the incident radiation on the pool surface with the fuel heat of gasification and smoke point. The ambient temperature, radiation level, side wind and vitiation of the atmosphere in situations of practical interest may significantly differ from those in experimental conditions. Furthermore, the transient nature of the analyses may require knowledge of the time-dependent burning rate, not just the peak or steady-state value.

Figure 2.4 illustrates the main heat transfer mechanisms in a burning liquid pool. The heat from the flame is transported to the liquid by thermal radiation and convection. Heat conduction takes place between the vessel and the liquid. The size of the pool dictates which mode of heat transfer dominates, although the type of fuel also plays a role [44,45]. For very small pool diameters, conduction through the vessel walls dominates the heat transfer. For slightly larger pool fires, convective transport is the primary mode, and for large pool fires, radiative transport dominates. The exact diameters at which these transitions between dominant heat transfer mechanisms occur are fuel dependent. For low sooting fires such as methanol, transition to the radiation dominated regime occurs at larger diameters compared to sootier fuels [47].

Figure 2.4 Heat transfer mechanisms in evaporation.

The capability of CFD models to predict the burning rates of liquid pool fires hinges on their ability to predict the heat feedback to the fuel surface. It is also not certain that the liquid side modeling capabilities in commonly used CFD software are up to the task. Wall-modeling for LES is also still an active research area. It is therefore necessary to develop sub-models for the CFD fire models that can predict the pool fire dynamics and burning rate during the simulation.

2.3.2 Pool fires in open atmosphere

Several authors have attempted to predict the burning rates of pool fires using either laminar or RANS equations fully coupled with the liquid phase. Prasad [48] solved
the laminar form of Navier-Stokes equations for a small 1 cm methanol pool fire. His model included heat transfer within the liquid by conduction but ignored in-depth radiation and convection. Snegirev et al. [17] predicted the burning rates of a wide range of acetone pool fires. They solved the Favre averaged governing equations together with the standard k-ε turbulence model. They used a Monte Carlo method to solve the weighted average of gray gases form of the RTE and included a model for turbulence radiation interaction. Novozhilov and Koseki [49] included one-dimensional heat transfer within the liquid in their model. The liquid evaporation rate was calculated based on a mass transfer calculation. They did not account for the blowing effect on the boundary layer. Pretrel et al. [18] attempted to reproduce the oscillatory behavior of a liquid pool fire in a mechanically ventilated compartment.

LES prediction of the pool burning rate of a methanol pool fire was performed by Hostikka et al. [50] In their model, the liquid evaporation rate was calculated iteratively over the course of the simulation to maintain an equilibrium fuel vapor pressure in the first gas-phase cell above the liquid boundary. The heat transfer inside the liquid layer was calculated using a one-dimensional heat conduction solver, ignoring the effects of convection and radiation. In the results, only the steady state burning rate value was observed, paying no attention to the temporal development. The main weakness of this kind of evaporation model is that the realized vapor concentration is highly sensitive to the spatial resolution.

Paper IV of this thesis presents simulations of an ethanol pool fire experiment conducted by Thomas et al. [51], who also reported simulations with FDS version 4. More recently, the same experiment was simulated using FDS version 6 [52]. They used the liquid pool boundary condition developed in this work. The evaporation model in FDS 4 maintained saturation pressure in the first grid cell above the evaporating surface, whereas in FDS 6 the evaporative mass flux is based on a mass transfer calculation. Despite the considerable differences in the evaporation models of FDS 4 and FDS 6, both models gave similar results. Neither model was able to reproduce the transient development of the burning rate.

In the light of the discussion in Section 2.1.4, the similarity in results of FDS 4 and FDS 6 is not surprising. Once the liquid heats up to a temperature near its boiling point, the boundary layer resistance to mass transfer is negligible and the evaporation rate is determined by prediction of incoming heat flux.

The mass transfer model developed in this thesis may be expected to differ from the equilibrium approach of FDS 4 in situations where the liquid temperature is below boiling point. These situations include pools evaporating in the absence of flame and liquid pool fires during the initial heat up phase. Modeling the evaporation in the latter case is likely to require detailed modelling of the internal heat transfer within the liquid.

In paper IV, we investigated the hypothesis that the slowly growing burning rate is related to heat transfer within the liquid fuel.
2.3.3 Pool fires in confined spaces

The burning rates in confined spaces, possibly coupled with mechanical ventilation, can be significantly different from those measured in open atmosphere. These differences are caused by e.g. air vitiation and heat radiation from hot walls and the hot gas layer. Empirical correlations have been proposed to relate the open atmosphere burning rate to the burning rate in compartments [53,54].

Suard et al. [55] related the total pool burning rate to the pool size and local oxygen concentration according to empirical correlations. Three experiments with hydrogenated tetrapropylene fuel in a mechanically ventilated compartment were used to validate the model. Wahlqvist and Hees used a similar methodology of modifying the experimentally observed burning rate for compartment fire conditions [56]. Such approaches cannot be considered to be fully coupled, since they still rely on knowledge of the burning rate in open atmosphere.

Ventilation systems may also give rise to a new kind of dynamics in the fire: burning rate oscillations [18,57]. The oscillatory phenomenon is explained as a coupling process between the heat release rate and inlet flow rate. These two variables are coupled through the compartment pressure. During oscillations, a phenomenon of “ghosting flame” is seen, in which the flame moves away from the pool and towards the air inlet. The prerequisites for the oscillatory phenomenon are under-ventilated conditions and high enough temperatures to allow combustion at low oxygen concentrations.

A numerical and experimental study was carried out by Pretrel et al. [18] on the oscillatory phenomenon. Simulations with the CFD code ISIS successfully predicted the two dominant low frequencies of the oscillatory behavior of the fuel MLR. However, the amplitude of the oscillations was substantially under predicted. FDS simulations of a heptane pool fire from the same set of experiments had similar results [58].

2.3.4 Heat transfer within the liquid phase

In the liquid phase of a pool fire, the dominant modes of transport are convection (fluid movement) and radiation. The heat to the surface is provided by conduction and convection from both the liquid phase and the gas phase. Therefore, the liquid side convection can have a major effect on the heat balance on the liquid surface.

There are several possible sources of fluid movement within the fuel. One source is the uneven burning rate of fuel, which will cause it to flow towards regions of high burning rates. The second source is the hot walls of the pool, where heat transferred through the pool walls creates natural convection currents. The third source is in-depth radiation absorption. During pool combustion, the pool surface is cooled by evaporation and the liquid is internally heated by absorption of radiation. Uneven heat flux to the liquid surface may also give rise to convective currents. Higuera [59] numerically explored a liquid layer with a cold bottom plate heated non-uniformly from above. For liquids with Prandtl numbers near unity, both thermocapillary and buoyant flows were induced.
Studies have also been conducted to determine the spectra of emitted radiation [60] and to characterize the radiation absorption by gases within the flame [61]. Heat transfer within the liquid phase of a pool fire has received less attention. In modeling efforts, the heat transfer is often ignored. In experiments, steps are often taken to minimize the effect of in-depth radiation absorption and convection. For example, rocks or glass beads may be placed in the fuel pan to reduce the heat transfer within the pool [47,62]. In [62], Suo-Anttila et al. investigated the effect of convection in the liquid phase by removing the rocks from the pan. They found the effect to be negligible. The in-depth absorption by semi-transparent fuels has been studied for PMMA [63], polymer films [64] and liquid pool fires [60]. Most of the research related to the in-depth radiation absorption in liquids considers the boil-over of liquid pool fires on water [65]. The effect of in-depth radiation absorption on evaporation of fuel droplets has also been studied [66].

Vali et al. at the University of Alberta conducted detailed studies of the liquid side convection in laboratory scale methanol pool fires [67–70]. They found that there is a nearly constant temperature region directly below the surface of a pool fire. In this region, convection driven by heated pool walls is the primary mode of heat transfer. They also noted that varying the temperature of the pool boundary affected the burning rate. The importance of the initial temperature of the liquid fuel on pool fire dynamics has been noted previously by Hayasaka et al. [71] and Chen et al. [72]. Chen et al. recorded the temperature gradient within the fuel. They found that the initial temperature affected the temporal development of the burning rate but did not significantly influence the steady state burning rate.

Depending on the fuel, the penetration depth of thermal radiation can vary considerably. In fuels that are optically very thick in the infrared region, a thin layer on the surface absorbs the majority of the thermal radiation. In this case, the radiation can be taken into account as a boundary condition of the liquid’s internal heat transfer problem. If the liquid is not optically thick, the in-depth absorption may need to be included as an internal source term of the heat conduction/convection problem. Additionally, the re-radiation of the fuel and vessel must be considered to ensure the conservation of energy in the case of optically thin fuels and high temperatures. In liquid spills, the layer thickness is often of similar magnitude or smaller than the absorption thickness in liquids.

2.4 Fireballs

Fireball may be defined as “fire, burning sufficiently rapidly for the burning mass to rise into the air like a cloud or ball.” [73]. Ignition of dust or vapor clouds or releases of flammable gases from pressurized containers will often result in a fireball. Various types of transportation accidents can also result in fireballs, as vessels containing liquid fuel burst and disperse their contents into the surrounding atmosphere. An important class of accidents that may result in a fireball are boiling liquid expanding vapor explosions (BLEVEs). A BLEVE occurs when a vessel containing pressurized
liquid is heated until it bursts [3]. The difference between a vapor cloud explosion and a fireball is that in fireballs there is little mixing of fuel and air before ignition.

Fireballs have relatively short lifetimes, during which they pass through three distinct stages: growth, steady burning, and burnout. In the growth phase, air is entrained into the fireball and the diameter, \( D(t) \), of the fireball increases. The rate of increase depends on the release type. If the fireball results from a high momentum release, such as pressurized vessel burst, \( D(t) \propto t^{1/3} \). If the fireball is buoyancy dominated, \( D(t) \propto t^2 \) [74]. During the steady state burning phase, the diameter of the fireball is relatively constant; the fireball begins to lift off and starts to form the familiar mushroom cloud shape. During the burnout phase, the fireball diameter remains the same, but the flame becomes translucent and finally disappears.

Knowledge of fireball size, duration, and height are critical for estimating the hazard caused by the fireball. Several empirical correlations exist for determining the diameters and lifetimes of fireballs. The review by Abbassi and Abbassi [3] is an excellent calculation methods used to model BLEVEs. These methods can also be used to analyze fireballs from aircraft impacts. However, they cannot be used to estimate the fraction of the unburnt fuel. Baum and Rehm [4] proposed a model for the global energy release rate of fireballs and used it to characterize the energy releases during the 2001 WTC attacks in New York. They used video footage from the attacks for calibrating the model. They concluded that only a fraction of the fuel carried by the planes burned in the initial fireballs. Thus, the majority of the aviation fuel was available to accelerate the fires in the buildings. Apart from the efforts of Baum and Rehm, the fraction of fuel left unburnt has not attracted much attention.

Large scale fireballs are difficult to study experimentally. As a result, very few well-documented experiments are available in open literature. The most commonly cited experiment was conducted by The Federal Institute of Material Research and Testing (BAM) in Germany [75,76]. They exposed a 45 m³ tank partially filled with 10 m³ of liquefied propane to an open pool fire. The resulting fireball was around 100 meters in diameter and had a duration of 7 seconds.

Numerical studies are much more common. Fireballs resulting from vertical fuel gas releases were investigated numerically by Makhlviladze et al [77]. Makhlviladze et al [78] extended this model to investigate two-phase fuel releases from pressurized containers of liquefied gas. Their model solves two-dimensional Favre-averaged Navier–Stokes equations by using the standard k-ε turbulence model and an infinitely fast one-step reaction. The dispersed phase is treated in a Lagrangian fashion. They assumed a monodisperse droplet size distribution with the initial velocities of the droplets derived from Bernoulli’s law. They compared the predicted lifetimes of fireballs with the experimental correlation of Roper et al. [79], and the transient shapes and sizes of the fireballs with the experiments of Hasegawa and Sato [80]. Makhlviladze [81] used this model to analyze total loss of containment scenarios for BLEVEs. They also investigated the overpressures that would occur in such events.

Yakush et al. [82] compared RANS and LES predictions of the fireball lifetime with the empirical correlation of Roper [79]. They used Fire Dynamics Simulator
(FDS) version 4 for the LES calculations. FDS was found to underestimate the fireball lifetimes. The fuel release was modeled with a gas inflow boundary condition. Hu [83] used a modified version of FDS to investigate deflagrations of premixed fuel vapor clouds. High-speed jets were not considered. Instead, the vapor clouds were created by slowly injecting gas into the simulation domain. Luther et. al. [84] used FDS version 5 to determine the spreading and extent of the fireball around a generic NPP. They also modeled the fuel insertion by using a gas inflow boundary condition. Shelke et al. [85] used FireFoam to simulate the fireball from the BAM BLEVE experiment and from a plane crash.

In the above fireball simulations, the fuel inlet boundary condition consisted of either a vertical spray or injection of fuel gas from a boundary patch. Initial velocities of the gas and droplets have been based on, for example, the theoretical calculations of flash evaporation. When multiphase models have been used, droplet sizes have been assumed to be monodisperse. The possibility of fuel droplets raining out of the fireball has usually been neglected. Ignoring the raining out of droplets may be justified because of the highly volatile nature of liquids such as liquefied natural gas (LNG) and propane that are being considered.

2.5 Numerical methods

2.5.1 Large eddy simulation

Due to the wide range of length scales present in a turbulent flow, direct solution of equations (1)-(4) is prohibitively expensive. For example, in a 1-meter wide pool fire with a heat release rate of 1 MW, the largest eddies are of the order of 0.5 m. On the other hand, the flame sheet thickness, which characterizes the length scale over which reactions occur, is of the order of 1 mm [86]. Such grid resolutions are not feasible with current hardware and will not be in the foreseeable future.

In large eddy simulation (LES), only the large energy-containing flow structures are resolved, and smaller structures are modeled. Formally this is achieved by low-pass filtering of the governing equations:

$$\bar{\phi}(x, t) = \int G(x - y)\phi(x, t)dy. \tag{17}$$

Here $\phi$ is a variable (such as pressure or velocity) and $G$ is a filter kernel. If density is not constant, Favre filtering $\bar{\phi} = \rho\bar{\phi}/\bar{\rho}$ may be used. The real value of a variable is then related to the value available in an LES by the relation $\phi = \bar{\phi} + \phi'$. Here $\bar{\phi}$ is the resolved, filtered value and $\phi'$ the unresolved fluctuation. The filtering operation is rarely applied explicitly. The numerical grid itself functions as a low pass filter and this is usually the only filtering considered.

As a result of the application of the low-pass filter, new unclosed terms appear in the governing equations. These are the product of applying the filtering operator to nonlinear parts of Equations (1)-(4). These new terms correspond to the effects of the unresolved scale on the solution, and their closures are called subgrid-scale
models (sgs models). The turbulent stress tensor is commonly closed with gradient diffusion type models
\[
\tau = \bar{u} \bar{u} - \bar{u} u = \nu_t S, \tag{18}
\]
where \( \nu_t \) is turbulent viscosity. Other models available for the subgrid scales stresses include models based on approximate-deconvolution, scale-similarity and Taylor expansion (see, e.g., [14,87])

In two-way coupled flows, the dispersed phase affects the large scales of the flow. The particles may enhance or modulate the turbulence. However, only a few researchers have proposed modifications to turbulence closures that account for the existence of the dispersed phase [88–92].

Finally, the filtered emission and absorption terms in the radiation transport equation need modeling. Often, the Optically Thin Fluctuation model is evoked allowing one to write:
\[
\vec{\kappa} I = \kappa \vec{I} \tag{19}
\]
However, the absorption-emission correlation \( \kappa T^4 \) cannot be ignored.

In addition to the terms discussed here, filtering of the governing equations also gives rise to unclosed terms in the governing equations of the dispersed phase. These terms will be discussed in Section 2.5.3.

### 2.5.2 Statistical description of spray

This section reviews the statistical framework that forms the basis for most spray models used in CFD codes. The theoretical framework provides justification for the spray models discussed in this thesis. The implications of the statistical description are discussed at the end of this section.

Williams [93] defined spray as any system of liquid or solid particles in a gas, where there are so many particles that only a statistical description of their behavior is feasible. All of the sprays considered in this thesis are included in this definition. One of the earliest attempts at complete statistical description of a spray is also due to Williams [94]. He derived an evolution equation for the droplet density function (ddf), defined as \( f(x,v,r,t) \). The density function describes the probability of finding a droplet within a volume of the phase space. The discussion of the spray equation here follows [95], see [96–99] for more detailed derivations.

Suppose that the spray is made up of an ensemble of \( N_s \) droplets which can all be described using \( M \) variables. The state of particle \( i \) is then represented by a vector \( \Phi_i^t = [\phi_1^i, ..., \phi_M^i] \). We then define the probability \( P(\psi,t) \) that describes the probability of finding a particle at position \( \psi \) in the phase space, e.g., a droplet with certain velocity and radius at a certain position, at a time instant \( t \). For the sprays considered in this thesis, the properties of the sprays can be described by position, velocity, radius and temperature of the droplets. The state space is then \( \psi = [V, R, T] \).

The modeled pdf is governed by the evolution equation
\[
\frac{\partial P}{\partial t} + \nabla \cdot [A(\mathbf{v}, r, T)P] + \frac{\partial}{\partial r} \left[ R(\mathbf{v}, T, r)P \right] + \frac{\partial}{\partial T} \left[ \dot{T}(\mathbf{v}, T, r)P \right] = 0
\] (20)

Here, \( A, R \) and \( \dot{T} \) denote the conditional expectation \( \langle \psi_j | \phi \rangle \) with \( \psi_j = V, R \) or \( T \). Here, \( \psi_j \) is the rate of change of property \( \psi_j \) and the brackets \( \langle \psi_j | \phi \rangle \) denote the expectation of \( \psi_j \) conditional on the particles being found in state \( \psi = \phi \).

Equation (20) is an exact, but unclosed, hyperbolic partial differential equation for the joint probability \( P(\phi, t) \). Due to the high dimensionality of the problem, the solution of Equation (20) with the usual finite volume and finite difference type methods is difficult. The equation is commonly solved using particle methods. If the continuous phase equations are solved in the Eulerian frame, the resulting method is called Lagrangian - Eulerian (LE). LE methods represent the spray by an ensemble surrogate of droplets \( \{X^{(i)}(t), V^{(i)}(t), R^{(i)}(t), 1 \ldots N(t)\} \). The properties of the surrogate droplets evolve according to:

\[
\frac{dX^{(i)}}{dt} = V^{(i)}
\] (21)

\[
\frac{dV^{(i)}}{dt} = A^{(i)}
\] (22)

\[
\frac{dR^{(i)}}{dt} = \dot{R}^{(i)}
\] (23)

\[
\frac{dT^{(i)}}{dt} = \Theta^{(i)}
\] (24)

Here, \( A^{(i)}, V^{(i)}, \dot{R}^{(i)} \) and \( \Theta^{(i)} \) are the modeled acceleration, velocity, vaporization rate and heating rate of the \( i \)-th surrogate particle. From the perspective of the work in this thesis, the main implications of the statistical description of sprays are [97,98]:

1. Primary atomization cannot be modeled with the spray equation that underlies LE methods. Instead, the initial spray needs to be described at a boundary where the primary atomization has finished.
2. The correspondence between real droplets in a spray and the surrogate droplets is only on the level of the conditional expected values. This gives considerable freedom in modeling the evolution equations of the surrogate drops. Particularly, this provides the possibility of using statistical models and adding random terms to the equations.
3. The point particle assumption has not been invoked in the derivation of Equation (20). As a result, Equation (20) is also valid for dense flows. LE methods can be used to model dense sprays. The influence of the volume fraction can be modeled through the expected drag.
2.5.3  Lagrangian-Eulerian particle models

In most engineering applications, the unsteady forces acting on a particle are negligible. The equation of motion of a rigid spherical particle is:

\[
\frac{dV^{(i)}}{dt} = \frac{\bar{u} - V^{(i)}}{\tau_p} + g \tag{25}
\]

Where the particle response time \(\tau_p\) is given by

\[
\tau_p = \frac{3}{2} \rho_p C_D \frac{\|\bar{u} - V^{(i)}\|}{\rho_p R^{(i)}} \tag{26}
\]

When solving Equation (25), we need to make some approximations. The first approximation is the continuous phase properties at the particle location, also called forward interpolation. The second is the method used to project the particle forces and mass source terms back to the Eulerian grid.

The most common approach for the forward interpolation is to use linear interpolation. However, simple linear interpolation does not preserve the divergence and curl of the interpolated velocity field. As inertial particles preferentially concentrate in regions of flow with high strain and low vorticity \([100]\), such interpolation errors could lead to errors in predictions of particle concentration.

Perhaps a more serious problem with the simple approach is that, in LES, only the low-pass filtered values \(\bar{u}\) are available. The fluctuating quantities \(u'\) need to be modeled. Bellan and O’Kong \([101]\) considered three types of models for the velocity seen by the particle: baseline, a deterministic and a stochastic model. Their baseline model directly utilized the low pass filtered velocity. Their assessment was that, for the purpose of calculating drop source terms, the random model performed most poorly and the deterministic model was the best.

Some authors have proposed Langevin-type equations for the fluid properties seen by the particle \([96,102,103]\). These models require solution of an extra set of ODEs for the fluctuating components.

Park et al. \([104]\) developed a dynamic subgrid-scale model for the velocity seen by the particle. They used an approximate deconvolution method together with a differential filter to estimate the unresolved velocity seen by the particles. They developed a dynamic procedure to determine the filter width \(\Delta\).

On the other hand, Bini and Jones \([95,96]\) developed a model for the acceleration experienced by a particle in turbulent flow. Their model could reproduce the non-Gaussian acceleration PDF’s observed in direct numerical simulations.
3. Methods

In this section, the methods used in the present work are reviewed. The simulation tool used in this thesis is the Fire Dynamics Simulator (FDS). The equations solved by FDS are reviewed in Section 3.1. The rest of this section reviews the modeling contributions from this thesis.

3.1 Description of the computational tool

3.1.1 Gas phase

FDS solves the Navier-Stokes equations in a form suitable for low-Mach number, thermally driven flows. The turbulence model in FDS is Large Eddy Simulation (LES). The low pass filtered equations of Low-Mach buoyancy-driven flow are given by [105]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = \dot{m}^\alpha
\]  

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{uu} = -\nabla \bar{p} + \nabla \cdot (\rho - \rho_0) \mathbf{g} + \mathbf{f}_b
\]  

\[
\frac{\partial \rho Y_{\alpha}}{\partial t} + \nabla \cdot \rho Y_{\alpha} \mathbf{u} = \nabla \cdot \mathbf{f}_\alpha + \dot{m}_{\alpha}^\alpha
\]  

\[
\frac{\partial \rho h_i}{\partial t} + \nabla \cdot \rho h_i \mathbf{u} = \frac{D \bar{p}}{D t} + \dot{q}^\alpha - \nabla \cdot \dot{q}^\alpha
\]  

\[
\tau = \rho (v + v_T) \left( (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}) \right)
\]  

\[
\dot{q}^\alpha = \rho c_p (k + k_i) \nabla T + \sum_{\alpha} \rho D a \nabla Y_{\alpha} + \dot{q}^\alpha_T
\]  

\[
\rho = \frac{\rho W}{RT} \quad W = \frac{1}{\sum_{\alpha} Y_{\alpha}/W_{\alpha}}
\]

Here the over bars denoting the low-pass filtering operation have been omitted for clarity. The low-Mach number approximation enables us to split the pressure into background pressure \( \bar{p} \) and perturbation pressure \( \tilde{p} \). Only the background pressure appears in the equation of state. Formally the low-Mach number equations can be derived from the compressible Navier-Stokes equations by expanding the variables in powers of the Mach number [106].

\footnote{Available form \url{https://pages.nist.gov/fds-smv/}}
Unless otherwise indicated, the turbulent viscosity is given a modified version of the model proposed by Deardorff [107]. The eddy viscosity is calculated from:

\[
\mu_t = \rho C_{dea} \Delta \sqrt{k_{sgs}}; \quad k_{sgs} = \frac{1}{2} ||u'||; \quad u' = \bar{u} - \bar{\bar{u}}.
\]  

(34)

Here \(\Delta\) is the filter width and \(C_{dea}=0.1\) is an empirical constant. The main difference between the above model and the usual one-equation turbulence closures is that the sgs kinetic energy is obtained by a scale similarity argument. In addition to the default Deardorff model, the dynamic Smagorinsky model [108,109] is also used.

3.1.2 Radiation

The contribution of thermal radiation to the energy equation is computed from

\[-\nabla \cdot \mathbf{q}'_{\text{r}} = \kappa (U - 4\pi I_{b}(\mathbf{x})); \quad U = \int_{4\pi} I(\mathbf{x}, \mathbf{s}') d\mathbf{s}'.\]

(35)

In the above, \(I(\mathbf{x}, \mathbf{s}')\) is the spectrally integrated intensity in the direction \(\mathbf{s}'\) at the location \(\mathbf{x}\), \(I_{b}(\mathbf{x})\) is the source term, and \(\kappa\) is the absorption coefficient. The intensity \(I\) is obtained as a solution to the radiation transport equation (RTE):

\[s \cdot \nabla I_s = [\kappa + \kappa_d + \sigma_a] I + \kappa I_{b} + \kappa_d I_{b,d} + \sigma_d \int_{4\pi} \Phi(s, s') I(\mathbf{x}, s') d\mathbf{s}'.\]

(36)

Here \(\kappa_d\) is the droplet absorption coefficient, \(\sigma_a\) is the droplet scattering coefficient, and \(I_{b,d}\) is the emission term of the droplets. The scattering phase function \(\Phi(s, s')\) gives the scattered intensity fraction from the direction \(s'\) to \(s\).

The mean absorption coefficient \(\kappa\) is tabulated as a function of the gas species and soot concentration by using the narrow-band model RadCal [110]. The absorption coefficient is given by

\[\kappa = \min[\kappa_p, \kappa_{eff}]\]

(37)

where \(\kappa_p\) is the Planck mean absorption coefficient, and the effective absorption coefficient is solved from

\[\int_{0}^{\infty} I_s (s) = \frac{\sigma}{\pi} \left[ e^{-\kappa_{eff} s T_{rad}} + (1 - e^{-\kappa_{eff} s T_{rad}}) T^{4} \right].\]

(38)

Here \(T_{rad}\) is the assumed temperature of incident radiation. It is taken to be 900 °C, corresponding to typical flame emission temperatures. The path length \(s\) is set to five times the nominal cell size. In engineering practice, the attainable grid resolutions are usually of the order of five grid cells across the plume. The effective mean absorption coefficient approaches the Planck mean absorption coefficient as the path length decreases. During simulations, the absorption coefficients are obtained by table lookup. The absorption and scattering coefficients of the liquid droplets are based on Mie theory [111]. The scattering integral is approximated as a sum of isotropic and forward components [112]. The RTE is solved using the Finite Volume Method for radiation [113].
As was discussed in Section 2.5.1, the source term in Eq. (36) requires modeling. In FDS the source term is computed as follows:

\[ I_b(x) = C \frac{\sigma T(x)^4}{\pi} C = \max \left[ 1, \frac{\int_{V} \rho \delta_T \sigma T^4 \, dv}{\int_{V} \rho \delta_T \, dv} \right] \] (39)

This method aims to ensure that the fraction of energy released from flames as radiation is globally equal to the radiant fraction \( \chi_r \).

### 3.1.3 Combustion

For all simulations in this thesis, the gas phase combustion is treated as a single step irreversible reaction of fuel and oxidizer:

\[ \text{Fuel} + \text{Air} \rightarrow \text{Products} \] (40)

The chemical heat source term in Equation (30) is given by

\[ \dot{q}^n = m_f^n \Delta h_c \] (41)

where \( \Delta h_c \) is the heat of combustion of the fuel. The rate of combustion is given by a model similar to the eddy dissipation concept (EDC) model [114]

\[ m_f^n = - \rho \min \left( \frac{\nu_f \omega_f}{\tau_{mix}} \right) \] (42)

where \( Y_f \) and \( Y_o \) are the mass fractions of the fuel and oxidizer, respectively. The mixing time scale \( \tau_{mix} \) is based on the local flow field [115].

FDS contains a simple extinction model based on the concept of critical flame temperature. For each computational cell, the extinction is determined by two criteria: The first rule suppresses the combustion if the temperature in the computational cell does not exceed a user defined auto ignition temperature. The second rule considers a stoichiometric pocket of fuel, air, and products in a computational cell. If the combustion energy of this fuel is not sufficient to increase the temperature of the gas mixture above the critical flame temperature, the combustion reaction is again suppressed. Both the critical flame temperature \( T_{CFT} \) and auto ignition temperature \( T_{AIT} \) are user-defined constants.

### 3.1.4 Evolution equations for the Lagrangian particles

FDS uses the LE method for the description of the dispersed phase. Buoyancy, lift, and forces arising from fluid acceleration are neglected. With these assumptions, the motion of a single computational droplet is governed by

\[ \frac{dV^{(i)}}{dt} = \tau_p^{-1} \left[ u^{(p)} - V^{(i)} \right] + g \] (43)

The drag coefficient \( C_D \) is given by
\[ C_D = \begin{cases} \frac{24}{Re} & \text{for } Re < 1 \\ 24(0.85 + 0.15Re_D^{0.687}) & \text{for } 1 \leq Re < 1000 \\ 0.44 & \text{for } 1000 \leq Re \end{cases} \] (44)

The mass of the particle evolves according to the pair of ODEs:
\[ \frac{dM^{(i)}_{\rho}}{dt} = Ah_m (\gamma_d^S - \gamma_{\rho,\rho}^{pp}), \] (45)
\[ M^{(i)}_{\rho} \frac{dT^{(i)}_l}{dt} = Ah (T_{\rho}^{g} - T^{(i)}_l) + \dot{q}_r + \frac{dM^{(i)}_{\rho}}{dt} \Delta h_v. \] (46)

As discussed earlier, each droplet represents several real droplets with the same properties. The fluid properties are interpolated at the droplet position using tri-linear interpolation. The backward interpolation is performed using a variant of the Particle-In-Cell (PIC) method, in which the mean particle source terms in Eqs (27)-(30) are calculated as the summation of the individual contributions of each particle in the control volume surrounding a grid node.

The quasi-steady drag approximation is employed here, and it can be justified on the grounds of the large density difference between the carrier phase and the dispersed phase. The grid resolutions used in most fire simulations are also too coarse to resolve the pressure gradients and mean shear forces in Eq. (8). The errors caused by the numerical discretization are likely to be much larger.

### 3.1.5 Condensed phase heat transfer model

The FDS condensed phase heat transfer model is used in modeling the liquid phase in papers IV and V. FDS calculates the heat transfer in the solid phase based on conduction and radiation. The model is applied on a cell-by-cell basis. This section describes the model as it is applied to liquid pool fires.

The FDS solid phase model solves the one-dimensional heat conduction equation for the liquid fuel given by
\[ \rho c_p \frac{dT_l}{dt} = \frac{\partial}{\partial x} \left[ k_l \frac{\partial T_l}{\partial x} \right] + \dot{q}^{m} \]
\[-k \left( \frac{\partial T_l}{\partial x} \right)_{S} = h(T_g - T_i^{s}) - \Delta h_v \dot{m}^{n} \]
\[ h = \max \left[ 1.52 |T_g - T_i^{s}|^{1/2}, \frac{k_g N_u}{L} \right] \] (47)

Here \( \rho, c_p, k_l, \) and \( \Delta h_v \) are the fuel density, specific heat, thermal conductivity, and evaporation heat, respectively. The subscripts \( l \) and \( g \) refer to the liquid and gas phases. The superscript \( s \) denotes the liquid surface.

The heat source term \( \dot{q}^{m} \) in Equation 47 accounts for the effect of the in-depth absorption of radiation and therefore radiation is not accounted for in the surface boundary condition. The radiation heat transfer within the one-dimensional layer is
calculated using a "two-flux" model in which the radiative intensity is assumed to be constant in the "forward" and "backward" hemispheres. The forward radiative heat flux into the fuel is

\[ \frac{dq^+}{dx} = \kappa(\sigma T^4 - \dot{q}^+) \]  \hspace{1cm} (48)

A corresponding formula can be written for the backward flux \( \dot{q}^- \). The heat source term in Equation 47 is the difference between the forward and backward fluxes

\[ \dot{q}^m = \frac{dq^+}{dx} - \frac{dq^-}{dx} \]  \hspace{1cm} (49)

Boundary condition at the fuel surface is given by

\[ \dot{q}^+|_{x=0} = \dot{q}^m_{in} + (1 - \varepsilon)\dot{q}^- \]  \hspace{1cm} (50)

where \( \varepsilon \) is the fuel emissivity and \( \dot{q}^m_{in} \) is the incoming radiative flux.

### 3.2 Spray modeling

#### 3.2.1 Overview

In order to correctly predict the spray dispersion, the characteristics of the initial spray must be accurately determined. This means that the droplet size distribution, initial velocity, and shape of the initial spray need to be described. For the present methodology, this means developing appropriate spray boundary conditions.

Section 3.2.2 discusses how to determine suitable droplet size distributions for use with the spray boundary conditions developed in Papers I and III.

Section 3.2.3 reviews the spray boundary condition for simulation of water mist sprays, developed in Paper I. Section 3.2.4 discusses the spray boundary condition for liquid dispersal from aircraft and liquid-filled projectile impacts, developed in Papers II and III.

Section 3.2.5 describes the three-way coupling model presented in Paper I. Additionally, Section 3.2.6 describes a turbulent dispersion model that was not presented in Papers I-V.

#### 3.2.2 Droplet size distributions

The classical approach for modeling the droplet size distributions is to fit an analytical distribution to the experimental data. Several choices for the droplet size distribution are available in the literature (see e.g. [116]). This thesis considers only three different analytical distributions: the Rosin-Rammler distribution, the lognormal distribution and the combination of the Rosin-Rammler and log-normal distributions. These three distributions were chosen because they are available for modeling the droplet size distributions in FDS.
The Rosin-Rammler distribution was initially developed for modeling the size distribution of coal particles, but has been widely used for modeling spray droplet size distributions [116]. The lognormal distribution is usually considered as a model for the Cumulative Number Fraction (CNF). Here it is used as a model for the Cumulative Volume Fraction (CVF) instead. The combination of these two distributions, called Rosin-Rammler-lognormal distribution, has been found to describe the droplet sizes in sprinkler sprays and is commonly used among fire safety engineers.

The Rosin-Rammler distribution is described by the CVF:

\[ F(d) = 1 - e^{-0.693 \left( \frac{d}{d_m} \right)^\gamma} \]  

CVF of the lognormal distribution is given by:

\[ F(d) = \frac{1}{\sqrt{2\pi\sigma}} \int_0^d \frac{1}{d'd'} \exp \left[ -\log\left( \frac{d'}{d_m} \right)^2 / 2\sigma^2 \right] dd' \]  

The Rosin-Rammler-lognormal combination:

\[ F(d) = \begin{cases} 1 - e^{-0.693 \left( \frac{d}{d_m} \right)^\gamma} & , d > d_m \\ \frac{1}{\sqrt{2\pi\sigma}} \int_0^d \frac{1}{d'd'} \exp \left[ -\log\left( \frac{d'}{d_m} \right)^2 / 2\sigma^2 \right] dd' & , d \leq d_m \end{cases} \]  

where \( d_m \) is the volumetric median diameter of the size distribution (half of the volume of the particles is in droplets smaller than this).

The numerical algorithm draws the droplet diameter from the cumulative number fraction (CNF), defined as

\[ f(d) = \frac{\int_0^d f_0(d')d'^{-3}dd'}{\int_0^\infty f_0(d')d'^{-3}dd'} \]  

Since the numerical algorithm picks the droplet sizes from the CNF, the CNF was also used in the parameter estimation in Papers I and II. The distribution parameters were found by least squares fit of Eq. (54) to the experimentally determined cumulative number distribution. The difference between using CVF or CNF for parameter estimation is that the former places more weight on large droplets, whereas the latter emphasizes the smaller drop sizes. This point was discussed extensively by Ditch et al. [117].

From the perspective of the work described in this thesis summary, it is important that the spray boundary condition is situated far enough from the nozzle so that all atomization processes have finished and the droplet distribution can be considered to be stable. Consequently, the droplet size distribution should also be determined sufficiently far from the spray inlet.

Ideally, the droplet size distribution would be determined at a position at which the breakup processes have finished but the entrainment into the spray and turbulent mixing has not had time to affect the measured distributions significantly.
However, finding this distance may be difficult. Measurements further away from the nozzle can be used if the effect of the entrainment and mixing on the droplet size distributions is taken into account. This can be done by using appropriate averaging of distributions measured at several positions.

Unlike the initial droplet size distributions, the initial velocities and flux densities should be determined as close to the location of the spray boundary condition as possible. Measurements of fluxes and velocities further away from the spray inlet can be used for validation.

3.2.2.1 Water mist nozzles

In Paper I, the droplet size distributions of three high-pressure water mist nozzles, called A, B, and C, were characterized based on data from NFPA750 characterization experiments. Measurements and the calculation of gross cumulative volume (GRV) distribution were in accordance with the NFPA750 standard, except that one measurement point was added in the center of the spray. The measured nozzles (called A, B, and C in Paper I) produced a relatively narrow cone with a dense core. The central point was included to capture this dense core of the spray better.

The GRV distribution was calculated as

\[
GRV(d_j) = \frac{\sum (R_{i,j} \times A_i \times v_i)}{\sum (A_i \times v_i)},
\]

(55)

where \(GRV(d_j)\) is the cumulative volume fraction of all droplets equal to or less than \(d_j\), and \(R_{i,j}\) is the cumulative volume fraction of droplets equal to or less than \(d_j\) at location \(i\). \(A_i\) and \(v_i\) are the cross-sectional area and the mist flux at location \(i\).

The Gross CFN was calculated similarly. The parameters for the Rosin-Rammler-Lognormal distribution (Eq. (53)) were found by least squares fitting of the CNF defined by Eq. (54). Table 3.1 lists the FDS simulation parameters for the A, B, and C nozzles from Paper I. The K-factor is based on manufacturer info, whereas the spread angle \(\theta\) was visually approximated from photographs of the spray.
Table 3.1 FDS Simulation parameters for nozzles A, B, and C from Paper I.

<table>
<thead>
<tr>
<th>Nozzle</th>
<th>K (l/min/bar³)</th>
<th>θ (°)</th>
<th>dₘ (µm)</th>
<th>γ</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.200</td>
<td>10</td>
<td>83</td>
<td>2.90</td>
</tr>
<tr>
<td>B</td>
<td>0.433</td>
<td>12</td>
<td>79</td>
<td>2.26</td>
</tr>
<tr>
<td>C</td>
<td>0.767</td>
<td>14</td>
<td>116</td>
<td>1.98</td>
</tr>
</tbody>
</table>

3.2.2.2 Sprays from liquid-filled missiles

The model is based on qualitative observations and quantitative characterization of the sprays resulting from high-speed impacts of water-filled missiles. Paper II describes the details of the experimental campaign and analysis methods. In this case, only a single measurement point was available. However, unlike the water mist sprays, the spray behavior was transient. Each experiment produced a slightly different droplet size distribution.

In all the tests, the spray concentration was found to follow a similar time dependence. The concentration peaks soon after the spray reaches the measurement position. A relatively long and dilute tail follows this initial front. Between 60% and 90% of the spray mass was found to pass the measurement position within the first 50 ms after the spray reached the measurement location.

Based on these observations, the experimental data was split into the “spray front” and “continuous” spray. In the analysis, the first 15 ms of the observations were assumed to belong to the spray front. The spray front contained approximately 20% of the total mass of the spray (approximated from measured volume fractions). The continuous spray is the rest of the spray. Table 5 shows the resulting size parameters.

The fitted distribution functions cannot capture all the features of the experimentally determined distributions. In particular, the experimental distributions had a sharp spike at the small particle diameters, followed by a long tail. The lognormal distribution function can reproduce this behavior most accurately. The Rosin-Rammler distribution significantly overpredicts the number of very small particles. In experiments SFP2-7, the continuous part of the spray contained large droplets, which increased the estimates of the volumetric median diameter dₘ.
Table 5. Fitted distribution parameters.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Experiment</th>
<th>Rosin-Rammler</th>
<th>Rosin-Rammler-Log-normal</th>
<th>Log-normal</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$d_m$ (μm)</td>
<td>$\gamma$</td>
<td>$d_m$ (μm)</td>
<td>$\gamma$</td>
</tr>
<tr>
<td>SFP 2.5</td>
<td>Whole</td>
<td>80</td>
<td>0.89</td>
<td>78</td>
</tr>
<tr>
<td></td>
<td>Front</td>
<td>90</td>
<td>1.03</td>
<td>87</td>
</tr>
<tr>
<td></td>
<td>Continuous</td>
<td>80</td>
<td>0.87</td>
<td>78</td>
</tr>
<tr>
<td>SFP 7.12</td>
<td>Whole</td>
<td>101</td>
<td>1.04</td>
<td>99</td>
</tr>
<tr>
<td></td>
<td>Front</td>
<td>84</td>
<td>1.42</td>
<td>82</td>
</tr>
<tr>
<td></td>
<td>Continuous</td>
<td>105</td>
<td>1.01</td>
<td>103</td>
</tr>
<tr>
<td>All</td>
<td>Whole</td>
<td>85</td>
<td>0.93</td>
<td>83</td>
</tr>
<tr>
<td></td>
<td>Front</td>
<td>88</td>
<td>1.09</td>
<td>85</td>
</tr>
<tr>
<td></td>
<td>Continuous</td>
<td>86</td>
<td>0.90</td>
<td>84</td>
</tr>
</tbody>
</table>

3.2.3 Spray boundary condition for water mist nozzles

As was discussed in Section 2.5.2, the Eulerian-Lagrangian particle model is not applicable in the solid region of the spray. Therefore, we did not attempt to model the atomization processes of the spray. Instead, we injected droplets to the simulation on a section of a spherical surface at distance $R$ from the nozzle. The section of the surface that launches the droplets is determined by the elevation angle $\theta$. Figure 3.1 illustrates the spray boundary condition. All atomization processes (primary and secondary) are assumed to have finished at this position. The size distribution of the inserted droplets then represents a stable size distribution, measured far from the spray inlet.

The spray boundary condition developed in Paper I assumes a Gaussian profile for the initial droplet volume fraction. Experimentally measured and predicted liquid volume fractions in a pressure atomized spray [21] achieve a Gaussian-like profile between 12.5 and 50 nozzle diameters from the inlet. If the spray boundary condition is very close to that of the jet inlet, the assumptions behind the Gaussian profile are less valid.

For large-scale simulations of fire suppression systems, it is critical that the spray boundary condition injects the correct amount of momentum along with the correct volume of water into the system. The momentum works as a driving force for large-scale mixing in the compartment. In Paper I, a simple relationship between the initial velocity of the droplet and the operating pressure of the nozzle was assumed:
\[ v_0 = C \sqrt{\frac{2p}{\rho}} \]  

(56)

Here \( p \) is the operating pressure of the nozzle, and \( \rho \) is the density of the liquid. In Paper I, we gave the discharge coefficient \( C \) the value 0.95. This value is not based on measurement and we did not carry out an extensive sensitivity analysis. All the droplets are given the same initial speed in the direction of the surface normal.

Note that the spray boundary condition defined here ignores deceleration of particles between the real injection point and the injection point in the simulation. The initial velocity defined by Eq. (56) ensures that the correct amount of momentum is injected into the simulation. Another approach would be to calculate the correct velocity of the droplets at distance corresponding to the spray boundary condition. In this approach, the gas phase velocity at the spray boundary condition should also be increased in order to conserve momentum.

The former approach is more complex than the one adopted in this thesis. The difference in the two approaches would likely be most important for small particles. However, small particles quickly reach their terminal velocity and therefore, the choice of using initial velocities defined by Eq. (56) simply causes the particle to slow down farther away from the nozzle than in reality. This effect is likely to be important only in the immediate vicinity of the spray boundary condition.
The initial position of a particle is picked randomly from the conical section described previously. The variable flux density within the spray is implemented by defining a probability density function for the initial position that depends on the latitude $\theta$ but not longitude $\varphi$. The joint probability of the initial latitude and longitude is

$$p(\theta, \varphi) = p(\theta)p(\varphi) = \frac{1}{2\pi} \sin \theta f(\theta)$$

(57)

Here the longitude is assumed to be independent of the latitude. If the function $f(\theta)$ is taken to be unity, the resulting mass flux is uniform. Prior to the implantation of the spray boundary condition in Paper I, FDS used uniform distribution to pick the latitude $\theta$. This corresponds to a flux distribution $f(\theta) = \sin \theta^{-1}$.

The exponential shape of the mass flux is implemented by using the probability density function

$$f(\theta) = \exp\left[-\beta \left(\frac{\theta - \theta_{\mu}}{\theta_{\max} - \theta_{\min}}\right)^3\right],$$

where

$$\theta_{\mu} = \begin{cases} 1/2(\theta_{\max} + \theta_{\min}) & \theta_{\min} \neq 0 \\ 0 & \theta_{\min} = 0 \end{cases}$$

(58)
The spread parameter $\beta = 5$ was chosen so that the simulations best fit the nozzle characterization experiments. In Paper I we did not attempt to provide a theoretical estimate for $\beta$. The following discussion is an addition to the discussion in Paper I.

For the case where $\theta_{\text{min}} = 0$ (full cone spray), an estimate for the spread parameter $\beta$ can be derived using the theory of turbulent round jets. We approximated the profiles of velocity and scalar density in a round jet with an exponential distribution

$$
c(x,r) = c_0 e^{\frac{-r^2}{2r_{1/2}^2}}.
$$

(59)

Here $r$ is the radial coordinate in the jet and $r_{1/2}$ is jet half-width. For a turbulent round jet, $dr_{1/2}/dx \approx 0.1 \ [13 \ p.111]$. The jet width at distance $x$ is then $r_{1/2} = x/10$. On the other hand, $r = x \tan \theta \approx x \theta$. Substituting gives

$$
c(x,r) = c_{\text{max}} e^{[-50\theta^2]} = c_{\text{max}} e^{[-50\theta_{\text{max}}^2 \left( \frac{\theta}{\theta_{\text{max}}} \right)^2]}.
$$

(60)

The estimate of $\beta$ is then $50\theta_{\text{max}}^2 = 2.37$. This is approximately half of the value used in Paper I. It is possible that nozzles A, B and C considered in Paper I place more water at the center of the jet by construction.

3.2.4 Spray boundary for liquid-filled missiles

Our model of an aircraft impact only describes the liquid dispersal from ruptured fuel tanks. The deformation of the missile and ejection of debris are ignored. The fuel dispersal process is modeled as a high-speed spray boundary condition. The model is based on qualitative observations and quantitative characterization of the sprays resulting from high-speed impacts of water-filled missiles [118].
Figure 3.2. Illustration of the spray boundary condition for aircraft impact simulations

Droplets enter the simulation at a randomly selected position on a spherical surface at distance R from the impact location. All droplets have the same initial speed, but the diameter of the droplets is randomly selected. Based on the analysis in Paper III, the initial speed of the inserted particles is 1.8 times the speed of impact.

Figure 3.2 illustrates the shape and parameters of the spray injection surface. The surface consists of two elements of a spherical surface, representing fuel released upwards and downwards. Visual observations from the Sandia experiments revealed that no fuel is released in the directions of the wings. The gaps in the injection surface account for the effect of the wings. The distance between the spherical surface and impact location should be greater than or equal to the characteristic length scale of missile deformation and primary liquid ejection. The particle distribution should represent a stable particle size distribution.

3.2.5 Three-way coupling between droplets and gas

As discussed in Section 2.5.3, in dense sprays the wakes behind individual droplets may start to influence other droplets. In Paper I, we presented a model for the drag reduction in dense sprays.

We base our model on the analytical formula developed by [119]. The model builds on the idea that in a configuration in which two particles with the same diameter are directly in line, the hydrodynamic force on the trailing particle can be calculated using drag correlations for an isolated sphere. However, the reference velocity in this calculation needs to be correctly defined. The authors employed the well-known analytical results for the wake of a sphere in laminar flow [119 p. 349]. They developed the following analytical formula for the hydrodynamic force to the second sphere.
\[ C_D = C_{D0} \frac{F}{F_0} \] (61)

where \( C_{D0} \) is the single droplet drag coefficient and \( F/F_0 \) is the hydrodynamic force ratio of trailing droplet to single droplet:

\[ \frac{F}{F_0} = \bar{W} \left[ 1 + \frac{Re}{16 \left( \frac{L}{d} - \frac{1}{2} \right)} \exp \left( -\frac{Re}{16 \left( \frac{L}{d} - \frac{1}{2} \right)} \right) \right], \] (62)

where \( Re \) is the single droplet-Reynolds number, \( L \) is the distance between the droplets and \( \bar{W} \) is the non-dimensional, non-disturbed wake velocity at the center of the trailing droplet

\[ \bar{W} = 1 - \frac{C_{D0}}{2} \left[ 1 - \exp \left( -\frac{Re}{16 \left( \frac{L}{d} - \frac{1}{2} \right)} \right) \right]. \] (63)

In our implementation, the separation distance \( L/d \) between droplet centers is calculated from the local droplet volume fraction, \( \alpha \), and local average droplet diameter \( \langle d \rangle \)

\[ \frac{L}{d} = \langle d \rangle \left( \frac{\pi}{6 \alpha} \right)^{\frac{3}{2}}. \] (64)

Eq. (64) gives the separation distance for evenly distributed spherical particles of diameter \( d \).

The hydrodynamic force predicted by Eq. (62) can be compared with the numerical results of Prahl et al. [121]. According to their study, Eq. (62) significantly underestimates the drag reduction at small drop-to-drop distances, where the wake is not fully developed, and (63) does not hold. At greater distances the two results are similar, the present correlation showing more drag reduction. The sprays considered in this paper are relatively dilute, and hence these short separation distances are not expected to be important.

### 3.2.6 Turbulent dispersion

Turbulent dispersion models were not used in Papers I-V. However, in Paper I, some features of the simulation results were credited to the turbulent mixing of particles. In this thesis summary, the effect of turbulent dispersion on water mist sprays is studied using the model developed by Bini and Jones [95,96]. The particle velocity evolves according to

\[ d\mathbf{V}^{(i)} = \tau_p^{-1} [\mathbf{V}^{(i)} - \mathbf{u}^{dp}] dt + g dt + \sqrt{\frac{k_{sgr}}{\tau_s}} d\mathbf{W}_t, \text{ with } \tau_s = \frac{v_t^2}{k_{sgr}} \] (65)

Here \( d\mathbf{W}_t = \sqrt{\Delta t} \xi \), with \( \xi \sim N(0,1) \), is an increment of the Wiener vector process. The subgrid scale kinetic energy is approximated from

\[ k_{sgr} = (\mu_t/\rho C_{dcr} \Delta)^2, \] (66)
This model is easy to implement, as it does not require the solution of additional ODEs for the turbulent velocity seen by the particle. Note that this model of turbulent dispersion is isotropic. Bini and Jones [95] developed an anisotropic version of the model, but this was not pursued here.

3.3 Modeling liquid pool fires

3.3.1 Mathematical model

The liquid pool fire model utilized in Papers IV and V is based on treating the liquid fuel as a semi-transparent solid with evaporation at the fuel surface. Heat transfer in the liquid is calculated using the condensed phase model in FDS, described in section 3.1.5. In Paper IV the earlier [50], equilibrium-based, mass transfer model was replaced by a mass transfer expression.

In Paper IV, the mass flux from the surface is calculated by a simple approach based on film theory. The molar flux in Eq. (13) can be related to mass flux using the ideal gas relation \( c = \frac{P}{RT} \).

The mass flux is then given by

\[
\dot{m}' = h_m \frac{\rho W_f}{RT} \log \left( \frac{X_f^p - 1}{X_f^S - 1} \right) ; \quad X_f^S = \exp \left( -\frac{\Delta \Delta n_W}{R} \left( \frac{1}{X_f^p} - \frac{1}{X_f^S} \right) \right) \tag{67}
\]

Here \( h_m = ShD_f/g/L \) is the mass transfer coefficient and \( \rho_f, g \) and \( X_f \) are the density of the fuel vapor and the volume fraction of fuel vapor in the grid cell adjacent to the pool surface, \( W \) is the molar mass of the fuel gas and \( R \) is the universal gas constant. \( D_f \) is the binary diffusivity of the vapor and the Sherwood number is given by

\[
Sh = 0.0375 c^{\frac{1}{2}} R^{\frac{1}{2}} ; \quad Re = \max \left[ 5 \cdot 10^5 \frac{\rho u L}{\mu} \right] . \tag{68}
\]

The Reynolds number is calculated based on the conditions in the cell adjacent to the surface. In the above, \( L \) is some characteristic length. Note that the Reynolds number is bounded from below, which ensures a non-zero mass flux from liquid fuels and thus circumvents the need to model the ignition process. The Reynolds number varies over time through the gas speed dependence, and so do the Sherwood and mass transfer numbers.

Papers IV and V did not present alternative methods for determining the mass transfer coefficient. In Paper IV, we briefly discussed the effect of mass transfer coefficient on predicted evaporation rates and concluded that because of the log term in Eq. (67), the importance of the mass transfer coefficient rapidly decreases as the liquid temperature approaches boiling point. The rest of this section adds to the discussion presented in Papers IV and V.

The Sherwood number in Eq. (67) and the Nusselt number in Eq. (47) represent average mass and heat transfer coefficients for a horizontal flat plate. The situation at the pool surface could perhaps more realistically be described as natural or mixed convection.

46
The use of flat plate correlations can be justified from two perspectives. Firstly, as discussed above, the mass transfer coefficient is important only in the initial phases of a pool fire, when surface temperature is far below boiling temperature. Secondly, the gas phase flow in pool fires is not driven by the temperature difference between the liquid surface and gas. Instead it is driven by heat generation outside the boundary layer. As such, the use of traditional natural convection based correlations is questionable. From the point of view of the pool surface, the situation is close to forced convection, where the entrainment in to the flame is driving the flow.

A simple alternative for the mass transfer coefficient can be derived using the viscous wall units given by Eq. (12). Assume that the non-dimensional film thickness $\delta^+$ is constant. The mass transfer coefficient can then be related to the non-dimensional film thickness by

$$\delta = \frac{\delta^+ v}{w}; h_m = \frac{\rho_s w_v}{\delta^+ v}.$$

We could, for example, assume that the film thickness is equal to the laminar sublayer thickness, $\delta^+ = 5$. However, in the following discussion $\delta^+$ is treated as a fitting parameter.

Figure 3.3 shows predicted evaporation velocities for toluene, calculated from Eq. (67). The mass transfer coefficient was calculated using Eq. (69). The black dots in Figure 3.3 correspond to the wind tunnel data of Reijnhardt and Rose [122]. In their experiments, they measured the evaporation rate of toluene in a wind tunnel. The pool was a square with 0.25 m side length. In their toluene evaporation experiments, the friction velocity derived from measurements directly in front of the pool was 0.43 m/s.

The fitting parameter $\delta^+ = 21.16$ produced the best fit to the data. The corresponding value of the mass transfer coefficient for this case is $h_m = 0.01$ m/s. The mass transfer coefficient used in Paper II gives $h_m = 0.034$ for this case.
Figure 3.3 The normalized evaporation rate of toluene as a function of temperature. The solid line is computed from Eqs. (67) and (69) with $D_F = 7.69 \times 10^{-6}$ m²/s (toluene at 20 ºC), $\nu = 1.50 \times 10^{-5}$ m²/s (air at 20 ºC) and $\delta^+ = 21$ (curve fit). Black dots correspond to experimental data from wind tunnel experiments [122,123] with $u_r = 0.43$ m/s.

The experimental data shows the importance of accounting for convective mass transfer. As the fluid temperature approaches boiling point, the mass flux increases exponentially. The log-term in Eq. (67) can capture this increase in evaporation rate quite well. This data was not used for validation of the evaporation model in Paper II and is reported here to highlight the effect of convection on mass transfer.

Note that the evaporation model used for droplets, Eq. (45), does not contain the logarithmic term appearing in Eq. (67). Figure 3.3 shows that the effect of blowing is only important near the boiling point. For the sprays considered in this thesis the liquids are injected at room temperature (20 ºC) and into similar ambient temperatures. Therefore, the effect of the logarithmic term is expected to be negligible.

The heat transfer coefficient in Equation (47) does not consider the effect of nonzero wall transpiration. The effect of blowing is to reduce the convective heat flux to the boundary [15]. The pool fires considered in this thesis are relatively large (0.5-3 meters in diameter), and radiation is the dominant heat transfer mode. For smaller pool fires the effect of blowing on convective heat transfer may have to be considered.

3.3.2 Effective absorption coefficients for in-depth radiation absorption

Absorption of thermal radiation in semi-transparent media is highly dependent on the wavelength of the radiation. A spectrally resolved (line-by-line) solution of Eq. (68) would be prohibitively expensive. It would also be unwarranted, as fire models often assume the gas to behave as a gray medium, and thus, the spectrum of incoming radiation is not known.
Paper II presents a method for determining effective absorption coefficients. The procedure is as follows:

1. Start with spectrally resolved absorption coefficients $\kappa_\lambda$ for a liquid.
2. Calculate the transmitted fraction of radiation at distance $x$ from the liquid surface by

$$
q^*_x(x) = \int_0^\infty q^*_{x,\lambda} (\tau) d\lambda
$$

(70)

$$
q^*_x = E_{b,\lambda}(T_\infty) 2E_2(\tau) + E_{b,\lambda}(T(x)) 2\int_0^\infty E_3(\tau') d\tau'
$$

(71)

Here, $\tau = \kappa x$ is the optical thickness, $T(x)$ and $T_\infty$ are the temperatures of the liquid and the external source. $E_{b,\lambda}(T_\infty)$ is the black body emissive power at wavelength $\lambda$.

$$
E_{b,\lambda}(T) = \frac{2hc^2}{\lambda^5} \frac{1}{\exp \left[ \frac{hc}{k_B T} \right] - 1}
$$

(72)

where $c$, $k_B$, and $h$ are the speed of light, the Boltzmann constant and the Planck constant, respectively. $E_2$ and $E_3$ are exponential integrals of the second and third kind, respectively.

3. Optimize to find a value for absorption coefficient $\kappa$ that minimizes some error metric between the predicted flux $q^*+$ from the solution of Eq. (48) and the flux calculated from Eq. (70).

Three choices need to be made in this process:

1. Choice of optimization metric.
2. The path length $L$ at which the flux $q^*$ is matched or over which the heat source distribution $q'''$ is matched.
3. The spectrum of the incoming radiation.

We investigated two optimization metrics in Paper II. The first one tries to produce an accurate flux at the bottom of the liquid layer $x = L$, thus giving a good estimate for the amount of energy absorbed by the liquid. The absorption coefficients corresponding to this criterion are given by:

$$
\kappa = \arg\min \left[ \frac{q^*(L)}{q^*(0)} - \frac{q'''(L)}{q'''(0)} \right].
$$

(73)

The absorption coefficients determined by the above criterion produce an accurate flux at the bottom boundary only at the beginning of the simulation. As the liquid layer thickness decreases, the flux will be increasingly inaccurate.

The second, alternative criterion attempts to reproduce the distribution of radiant flux over the entire thickness of the liquid layer. This choice should provide more accurate distribution of temperature inside the liquid, but it may not conserve the
energy as well as the first criterion. The absorption coefficients corresponding to the second criterion are given by:

$$\kappa = \arg \min \left[ \int_0^L \left( \frac{\alpha(x)}{\alpha_{\text{ref}}} - \frac{\alpha(x)}{\alpha_{\text{ref}}} \right)^2 \, dx \right]. \quad (74)$$

This second criterion is less sensitive to the choice of the path length $L$ than the first.

In Paper II, the former method was termed M1 (for Method 1), and the latter was named M2 (Method 2). Figure 3.4 shows the transmitted fraction of radiation as a function of path length for liquid heptane. The continuous black line corresponds to the solution of Eq. (70). The dotted line shows the predicted flux $\dot{q}^*$ from solution of Eq. (50) using the two different methods of determining the absorption coefficient.

Figure 3.4 Left: Results from a simulation of radiation transport in heptane. Comparison of line-by-line solution and the two approaches for determining the effective absorption coefficient. Right: The absorption coefficient spectra of heptane with black body emissive power imposed (in red).

Figure 3.4 shows that neither method of determining the absorption coefficient can reproduce the exact attenuation of radiation predicted by Eq. (70). In order to correctly capture the long tail of the attenuation, the wavelength dependency of radiation would need to be addressed in some way. The line-by-line solution in Figure 3.4 also shows that for heptane, most of the absorption of thermal radiation takes place within 4 mm of the fuel surface. However, a fraction of the incoming radiation (approximately 10% for heptane) may penetrate deep into the liquid layer.

### 3.3.3 Modeling the effects of convection in the liquid phase

As discussed in Section 2, accurate description of the liquid phase in pool fires would require solving the full Navier-Stokes equation with radiation heat transfer within the liquid. Such an approach is very complex and time-consuming. In Paper II, we explored an alternative approach of adjusting the thermal conductivity to take into account the internal convection. The Nusselt number gives the non-dimensional heat flux due to convective and conductive motions at an arbitrary plane in the liquid:

$$Nu = \frac{\dot{q}^\text{conv}}{\rho C_p \kappa \Delta \tau} \quad (75)$$
If we assume that heat conduction can model the heat transfer by convection with an effective conductivity $k_{\text{eff}}$, Eq. (75) becomes

$$ Nu = \frac{k_{\text{eff}}}{k}. $$ (76)

In Paper IV, we assumed that in large pool fires the primary source of convective motions is buoyancy generated by in-depth radiation absorption. We then calculated an effective thermal conductivity that reproduces the heat flux through the liquid layer at the surface of the fuel. We calculated the Nusselt number from a correlation for an internally heated horizontal plane layer with an isothermal top boundary and a thermally insulated bottom boundary[124]:

$$ Nu = 0.338Ra^{0.227}. $$ (77)

Here $Ra_i$ is the internal Rayleigh number:

$$ Ra_i = \frac{g \beta q'' H^2}{k \alpha}. $$ (78)

where $\beta$ is the coefficient of thermal expansion of liquid, $q''$ is the volumetric heat source and $H$ is a characteristic length scale. In the denominator, $\alpha$ is the thermal diffusivity of the liquid. Correlation (78) is derived for a case in which the internal heating is uniform. However, heat source distribution due to the absorption of radiation is approximately exponential. A Rayleigh number corrected for this distribution type is given by [125]

$$ Ra_{i,corr} = \frac{g \beta q'' H^2 \eta^2}{k \alpha} \left[ 1 - \left( \frac{1}{\eta} \right) \exp \left( -\frac{1}{\eta} \right) \right]. $$ (79)

Here $\eta = 1/\kappa$ is the length scale associated with the source distribution. The normalization constant $Q(\eta)$ in Eq. (79) is calculated from

$$ Q(\eta) = \int_0^\eta \exp \left( -\frac{z}{\eta} \right) dz = \eta \left[ 1 - \exp \left( -\frac{\eta}{\eta} \right) \right]. $$ (80)

The effective thermal conductivity model described above is likely to work better for relatively thin layers of fuel. In thin layers, convection can be thought to cause mixing through the whole layer. In deeper pools, the convective currents are likely to involve only a part of the liquid. Table 3.3 lists the thermophysical properties of the liquid considered in Paper II.

Table 3.2 gives calculated Nusselt numbers for the situation considered in Paper IV (Table 5). For this case $q'' = 20 \text{ kW/m}^2$ and the layer thickness $H$ is 1 cm. It can be seen that for most liquids the Rayleigh numbers are $O(10^7)$ and the Nusselt numbers are $O(10)$. Therefore, we conclude that the heat transfer through the fuel would be greatly enhanced by convection.

A significant source of uncertainty in calculating the effective thermal conductivity is the characteristic length scale. We take the characteristic length $H$ to be the depth of the liquid layer, which is constantly changing as the fuel is consumed. Furthermore, Eq. (78) also depends on knowing the volumetric heating rate.
Table 3.2 Nusselt numbers calculated from Eqs. (77)-(80). $Ra_i$ is the internal Rayleigh number for uniform heating given by Eq. (78). $Ra_{corr}$ is the corrected Rayleigh number given by Eq. (79).

<table>
<thead>
<tr>
<th>fuel</th>
<th>$\kappa$ (1/m)</th>
<th>$\eta$ (mm)</th>
<th>$Ra_i \times 10^3$</th>
<th>$Ra_{corr} \times 10^7$</th>
<th>Nu based on $Ra_i$</th>
<th>Nu based on $Ra_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>1000</td>
<td>1</td>
<td>1.6</td>
<td>1.6</td>
<td>25</td>
<td>15</td>
</tr>
<tr>
<td>Ethanol</td>
<td>1140</td>
<td>9</td>
<td>1.1</td>
<td>0.99</td>
<td>23</td>
<td>13</td>
</tr>
<tr>
<td>Water</td>
<td>1345</td>
<td>7</td>
<td>5.9</td>
<td>0.044</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>Benzene</td>
<td>162</td>
<td>6</td>
<td>2.1</td>
<td>7.9</td>
<td>26</td>
<td>21</td>
</tr>
<tr>
<td>Heptane</td>
<td>335</td>
<td>3</td>
<td>3.4</td>
<td>8.8</td>
<td>29</td>
<td>22</td>
</tr>
<tr>
<td>Toluene</td>
<td>289</td>
<td>4</td>
<td>2.2</td>
<td>6.3</td>
<td>26</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 3.3 Thermophysical parameters of the liquids considered.

<table>
<thead>
<tr>
<th></th>
<th>$k$</th>
<th>$\nu$</th>
<th>$\beta$</th>
<th>$\rho$</th>
<th>$c_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>W/m</td>
<td>m$^2$/s 10$^{-2}$</td>
<td>1/$k$ 10$^{-3}$</td>
<td>kg/m$^3$</td>
<td>kJ/kg K</td>
</tr>
<tr>
<td>Heptane</td>
<td>0.14</td>
<td>5.57</td>
<td>1.24</td>
<td>675</td>
<td>2.24</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.17</td>
<td>13.9</td>
<td>1.09</td>
<td>789</td>
<td>2.72</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.20</td>
<td>7.08</td>
<td>1.18</td>
<td>791</td>
<td>2.51</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.15</td>
<td>6.34</td>
<td>1.08</td>
<td>867</td>
<td>1.72</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.17</td>
<td>6.88</td>
<td>1.25</td>
<td>873.8</td>
<td>1.92</td>
</tr>
<tr>
<td>Water</td>
<td>0.58</td>
<td>8.9</td>
<td>0.21</td>
<td>1000</td>
<td>4.19</td>
</tr>
</tbody>
</table>

The corrected Rayleigh number in Eq. (79) is based on non-dimensional analysis, in which all length scales are scaled by the liquid layer height $H$. The length scale $\eta$ used in Paper IV (Eq. (81)) is not normalized. Using a normalized length scale $\eta = 1/kH$, the normalization constant $Q(\eta)$ in Eq. (79) is calculated from

$$Q(\eta) = \int_0^1 \exp \left[-\frac{z}{\eta}\right] dz = \eta \left[1 - \exp \left(-\frac{1}{\eta}\right)\right].$$  (81)

Table 3.4 compares the Rayleigh numbers and Nusselt numbers calculated using the normalized length scale. The Nu values calculated here are approximately three times higher than those calculated in Paper II. This does not affect the conclusions of Paper II, as the order of magnitude remains the same.
Table 3.4 Nusselt numbers calculated from Eqs. (77)-(79) and (81). \( Ra_{\text{corr,new}} \) is the corrected Rayleigh number given by Eq. (79) and the normalization constant given in Eq. (81). \( Nu_{\text{orig}} \) is the Nusselt number calculated using the original normalization constant given by Eq. (80).

<table>
<thead>
<tr>
<th>fuel</th>
<th>( \kappa ) (1/m)</th>
<th>( \eta ) (%)</th>
<th>( Ra_{\text{corr,new}} \times 10^7 )</th>
<th>( Nu_{\text{orig}} )</th>
<th>( Nu_{\text{new}} )</th>
<th>( Nu_{\text{orig}} / Nu_{\text{new}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heptane</td>
<td>335</td>
<td>0.30</td>
<td>8.83</td>
<td>7.9</td>
<td>21.5</td>
<td>2.7</td>
</tr>
<tr>
<td>Ethanol</td>
<td>1140</td>
<td>0.09</td>
<td>0.992</td>
<td>4.6</td>
<td>13.1</td>
<td>2.8</td>
</tr>
<tr>
<td>Methanol</td>
<td>1000</td>
<td>0.10</td>
<td>1.59</td>
<td>5.1</td>
<td>14.6</td>
<td>2.8</td>
</tr>
<tr>
<td>Toluene</td>
<td>289</td>
<td>0.35</td>
<td>6.27</td>
<td>7.4</td>
<td>19.9</td>
<td>2.7</td>
</tr>
<tr>
<td>Benzene</td>
<td>162</td>
<td>0.62</td>
<td>7.95</td>
<td>8.7</td>
<td>21.0</td>
<td>2.4</td>
</tr>
<tr>
<td>Water</td>
<td>1345</td>
<td>0.07</td>
<td>0.04</td>
<td>2.3</td>
<td>6.4</td>
<td>2.8</td>
</tr>
</tbody>
</table>
4. Results and discussion

4.1 Overview

This section includes a summary of the most important results described in Publications I-V and some additional results that provide more insight into the results reported in the Papers. The published results are divided into Spray modeling, Liquid pool fire modeling, and Risk analysis. For each subject, the results are divided into verification, validation, and application.

The verification of computational software is a process in which an attempt is made to ascertain the quality of the implementation. The verification can be performed by calculating simple problems for which an analytical solution is known. The validation of a model is the process in which the predictions of the model are compared with experiments, and the predictive uncertainty is quantified.

One could argue that if the model agrees well with experimental results, this should be seen as proof that the model is correctly implemented. However, invariably there are discrepancies between the model predictions and experimental results. It is then important to determine whether this is due to inaccuracies in the models themselves or to their incorrect implementation. It is also possible that good results can be obtained even after an incorrect implementation of a model. In each case, incorrect conclusions will be drawn concerning the capability of the model. Therefore it is important to consider both verification and validation.

In Paper I, we validated the basic implementation of the LE method in FDS using data from high-pressure water mist experiments. We investigated the capability of FDS to predict the drop size, velocity, droplet flux and number concentration profiles within the spray cone. The effects of turbulence modeling on the predictions of the spray dynamics were assessed. Prediction of air entrainment by high-speed water sprays was validated using experiments in rectangular channels with open ends. In Paper III, the spray boundary condition for aircraft and liquid missile impacts was developed. Predictions of liquid front velocities were compared with experimental results. Predicted spray shapes were visually compared with still images from experiments.

Paper III presented an application of the developed models for risk analysis. As a contribution to the validation work, Paper III compared the predicted lifetimes and diameters of fireballs from two-phase releases.

In Papers IV and V we presented validation of the pool evaporation model. Paper IV considered pools in the open atmosphere and investigated the effects of in-depth heat transfer on temporal development of the burning rate. Paper V focused on pool fires in mechanically ventilated compartments. Paper V also compared the predicted temperatures in the liquid phase of a pool fire with experimental observations.

This thesis summary also reports some additional results, that were not included in Papers I-V. These additional results are the verification tests and results from the turbulent dispersion model described in section 3.2.6.
4.2 Spray modeling

4.2.1 Verification

The verification of the particle tracking solver in FDS involves checking that the two-way coupling between the phases works correctly. The momentum transfer between particles and gas is verified by test cases that consider a 1 m by 1 m by 1 m channel with periodic boundary conditions on the x-faces and FREE_SLIP walls on the y- and z-faces. Static droplets are placed in the center of the channel, so that they form a surface perpendicular to the flow direction. Gravity is set to zero.

Assuming that the droplets are of uniform diameter and the drag coefficient and gas density are constant, the velocity in the channel decays according to

\[
\begin{align*}
  u &= \frac{u_0}{1 + Br u_0^2}, \\
  B &= \frac{1}{2} \sum C_D \pi r_d^2 V.
\end{align*}
\]

(82)

where \( V \) is the volume of the channel, \( r_d \) is the droplet radius, and \( u \) is the gas velocity in the x-direction. The summation is over all N particles. The common parameters used in all the simulations are: \( C_D = 10, r_d = 0.005 \text{ m} \).

Table 4.1 lists the initial velocities, \( u_0 \) and particle numbers. Figure 4.1 shows comparisons of computed and analytical results, indicating that the current integration scheme accurately predicts the amount of momentum transferred from droplets to the gas phase. The FDS verification suite includes this case (with the name particle_drag_A-F). In cases A-C there is one particle per computational cell, while in cases D-F there are ten.

Table 4.1. Parameters for the particle momentum transfer tests.

<table>
<thead>
<tr>
<th>Case</th>
<th>( u_0 )</th>
<th>( N )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>10</td>
<td>16</td>
</tr>
<tr>
<td>B</td>
<td>50</td>
<td>16</td>
</tr>
<tr>
<td>C</td>
<td>100</td>
<td>16</td>
</tr>
<tr>
<td>D</td>
<td>50</td>
<td>1600</td>
</tr>
<tr>
<td>E</td>
<td>100</td>
<td>1600</td>
</tr>
<tr>
<td>F</td>
<td>150</td>
<td>1600</td>
</tr>
</tbody>
</table>
Another simple verification test is prediction of the particle terminal velocity. The particle reaches its terminal velocity when the drag force and gravitational force exactly match, leading to velocity:

$$V_{\text{term}} = \sqrt{\frac{2m_p g}{\rho A_{\text{eff}} C_d}}$$  \hspace{1cm} (83)

This equation needs to be solved implicitly, since, especially for small droplets, the terminal velocity is low, and the corresponding drag coefficient is non-linearly dependent on the velocity.

Table 4.2 lists errors in terminal velocity predictions for a range of particle sizes. There is a significant error in predicting the terminal velocities of very small droplets. The integration method employed in FDS holds the drag coefficient constant over a time step. When Re<1, as is the case for droplets smaller than 100 µm, drag coefficient varies rapidly as a function of velocity. The terminal velocity of very small droplets is also low. The uncertainty in predicting the gas phase velocity is likely to be an order of magnitude greater than the error in the terminal velocity. This verification case is slightly modified from the particle terminal velocity (terminal_velocity) case in FDS verification suite.

Table 4.2 Error in terminal velocity predictions.

<table>
<thead>
<tr>
<th>d (µm)</th>
<th>Re</th>
<th>$V_{\text{term}}$ Eq. (59)</th>
<th>$V_{\text{term}}$ FDS</th>
<th>error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.14E-06</td>
<td>3.12E-05</td>
<td>1.99E-03</td>
<td>6288</td>
</tr>
<tr>
<td>10</td>
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<td>3.03E-03</td>
<td>1.76E-03</td>
<td>-42</td>
</tr>
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<td>100</td>
<td>1.87E+00</td>
<td>2.80E-01</td>
<td>2.81E-01</td>
<td>&lt;1</td>
</tr>
<tr>
<td>1000</td>
<td>2.62E+02</td>
<td>3.92E+00</td>
<td>3.93E+00</td>
<td>&lt;1</td>
</tr>
<tr>
<td>10000</td>
<td>1.05E+04</td>
<td>1.57E+01</td>
<td>1.58E+01</td>
<td>&lt;1</td>
</tr>
</tbody>
</table>
4.2.2 Simulation of nozzle characterization experiments

The NFPA 750 nozzle characterization experiments in Paper I were modeled using a rectangular computational area 1.5 m high, 0.5 m wide and 0.5 m deep. The computational area was open on all sides. The nozzles were placed 0.1 m from the top of the computational domain, and the measurements were made 1 meter below the nozzle. The simulation results corresponded to droplet properties averaged over a sphere with 1 cm radius centered at the measurement location.

FDS is a continuously developed code, and the simulation results in Paper I are several years old at the time of writing this thesis. For this reason, the simulations have been rerun with a newer version of the code. There are some small differences in the results, but the conclusions made in Paper I still hold. Here, only results for nozzle B are shown. The results for the other nozzles are similar.

Figure 4.2 shows a grid convergence study for mean drop velocity, droplet flux and mean drop size $d_{10}$. In Paper I, discretization intervals of 1, 2 and 4 cm were investigated. Here, the simulations were also carried out with a 0.5 cm discretization. The spatial resolution had a strong effect on the simulation results. In Paper I, the difference between 1 and 2 cm discretization intervals was deemed insignificant, but there was a considerable difference between 4 cm and 2 cm grids. However, Figure 4.2 shows that results on a 0.5 cm grid differ significantly from those on the 1 cm grid. The results on 0.5 cm grid are within experimental uncertainty. However, the large difference in results on the two finest grids points to issues with grid convergence. Section 4.2.5 discusses this issue in more detail.

The velocities and fluxes tend to be over-predicted except on the finest grid. In Paper I, this effect was attributed to the turbulence model and especially to the increased turbulent dispersion of particles when using the Dynamic Smagorinsky model.

A distinct feature of the experimental data is the flat diameter profile. Entrainment into the spray tends to produce a V-shaped profile of average diameter. Smaller droplets have shorter response times and are quickly drawn into the center of the jet. The FDS simulations with the default Deardorff model predict the usual V-shaped average diameter profile.
Figure 4.2 Comparison of predicted and experimental velocity, droplet flux and average diameter profiles in the NFPA tests of micro nozzle B from Paper I. Recreated here using FDS version 6.5.3 and the Deardorff turbulence model.

The sensitivity of the results to the initial velocity and the offset parameter was also investigated. Initial velocity could be varied at least 10% without a significant impact on the results. Varying the offset parameter between 5 cm and 15 cm also had a negligible effect.

4.2.2.1 Effect of the drag reduction model

We investigated the effect of the drag reduction caused by three-way coupling on the water spray characteristics by running the nozzle characterization tests with and without the drag reduction model described in Section 3.2.5. The model had a very modest effect on the results. The most noticeable effect was a slight flattening of the droplet diameter profile when the drag reduction model was included. The droplet volume fractions in the densest parts of the spray were just slightly over $\alpha>0.01$ for all nozzles. These results indicate that droplet-droplet aerodynamic interactions are not significant in modeling water mist systems created with the nozzles of this study. The drag reduction model was used in all simulations of Paper I.
4.2.2.2 Effect of the turbulent dispersion model

In Paper I, the dynamic Smagorinsky model was found to perform better than the default Deardorff model. The better performance of the dynamic Smagorinsky model was attributed to the increased gas phase mixing with the model. Here this hypothesis is further investigated. The turbulent dispersion model described in Section 3.2.6 was implemented in FDS version 6.5.3.

Figure 4.3 shows the velocity, diameter and mist flux profiles in the NFPA characterization experiments with and without the turbulent dispersion model. The model has only a modest effect on the velocity profiles. The relative velocity between the droplets and the gas quickly relaxes towards the terminal velocity of the droplets. Further away from the nozzle, the jet motion is driven by the gas momentum, and the droplets act as tracers.

The turbulent dispersion model has a greater effect on the droplet flux curves and average diameter profiles. The dynamic Smagorinsky model and the turbulent dispersion model together with the Deardorff model have similar effects. On coarse grids the flux profiles are flattened but, as the grid is refined, the flux profiles converge towards the experimental data. Notably, models produce a flatter diameter distribution compared to the default Deardorff model (See Figure 4.2). This provides more evidence that the flat diameter distributions observed for nozzles A, B and C are caused by turbulent mixing of the droplets, with smaller droplets being more easily ejected from the core of the spray.

The results presented in this section support the conclusions made in Paper I. The differences between the Deardorff model and the dynamic Smagorinsky model are to a great extent caused by increased turbulent dispersion of droplets when the latter model is used. An advantage of the turbulent dispersion model investigated here is that it is computationally cheaper than the dynamic Smagorinsky model.
Figure 4.3 Comparison of predicted and experimental velocity, droplet flux and average diameter profiles in the NFPA tests of micro nozzle B from Paper I. On the right, results using the Dynamic Smagorinsky model. On the left, results using the Deardorff model and the turbulent dispersion model described in Section 3.2.6.

4.2.3 Air entrainment

Correct prediction of air entrainment is crucial for predicting the penetration capability of water mist sprays. The air entrainment results indicate the accuracy of simulations in which the capability of the water mist to penetrate to the vicinity of the fire and to mix the gas space is important. Air entrainment into sprays is also important for predicting the dispersion of liquids from liquid jets. Small droplets
behave almost as flow tracers. The air entrained into the spray jet carries the droplets further than they could travel on their own.

The multi-orifice nozzles were modeled by positioning several single orifice models with different orientations at one point in the computational domain. The center nozzle points in the axial direction and the perimeter nozzles are equally spaced and at the same angle in relation to the center nozzle. The smaller the perimeter angle, the more parallel are the orifices in the spray head. Details can be found in Paper I.

Comparisons of the air entrainment simulations to the experimental results are shown in Figure 4.4. Figure a) shows the centerline velocities for the single-orifice spray heads. The center line and close-to-the-wall velocities for the multi-orifice spray heads are shown in Figures b and c, respectively.

Of the single-orifice nozzles, the entrainment for nozzle B is predicted within the experimental uncertainty. For nozzle C, the velocities in the channel are overestimated by about 20%, and for nozzle A the velocities are underestimated by a similar amount. For the multi-orifice spray heads, the agreement with the experiment is good on the centerline of the channel. The difference between these spray heads is the amount of x-momentum injected into the simulation.

![Figure 4.4](image1.png)

**Figure 4.4** Comparison of measured and predicted velocities in the air entrainment tests. Velocity at the channel center for single orifices in a). Center and wall velocity for multi-orifice heads in b) and c). Random noise is introduced to x-values to avoid symbol overlap.
4.2.4 Liquid sprays from missile impacts.

In paper III, the FDS spray model was validated both by quantitative comparisons of the spray front velocity data and qualitative comparisons of spray shapes. Details of the simulation models can be found in Paper III. Details of the experiments and analysis of the experimental results can be found in Paper II.

Figure 4.5 compares the predicted spray front velocities to the velocities determined from experiments. The shaded areas in the graphs correspond to the minimum and maximum velocities at a given time instant, while including experimental uncertainty (+/-25 m/s). The circles represent the median velocity from all directions. The predicted velocities were close to the median of the experimentally observed velocities. Near the impact location, the propagation velocity tended to be overestimated. This behavior can be explained by the effect of the missile fragments on the propagation of the jets.

The spray propagation velocity was highest in the directions in which it was unimpeded by shell fragments. The spray boundary condition does not account for projectile fragments; therefore the simulated liquid front propagation velocities were more closely related to the maximum (unimpeded) liquid front velocities. In cases in which the missile deformation had a smaller effect, the predicted liquid front velocities were close to the median velocity.

Further away from the impact location, entrainment into the individual jets caused the jets to spread and merge with nearby jets. This merging smoothed the edge of the spray pattern and consequently decreased the variability in propagation speed between directions. Therefore, the good correspondence between the simulation and the median velocities at later stages indicated that the entrainment in the sprays was correctly predicted.

The results show that the sprays from missile impacts can be simulated using the same methods as are used in simulations of water mist sprays. When the droplet size and initial velocity were correctly prescribed, the spray propagation predictions fell within the range of experimental uncertainty. This was true especially far away from the impact location, where the effects of missile fragments on spray propagation had diminished. Note that the initial velocity estimate was derived from the same experimental data that was used for the validation of the spray front propagation experiments. It is unclear whether this relation holds for other missile impact scenarios.
4.2.5 Grid resolution requirements

Grid resolution is perhaps the most important parameter in a CFD study. In LES, the grid should be fine enough to resolve the so-called "energy-containing eddies". In LES, the filter width should lie well within the inertial subrange of the kinetic energy spectrum. The existence and location of the inertial subrange are not known a priori. Using arguments based on model spectra of isotropic turbulence, Pope [14,126] showed that if the SGS model corresponds to under 20% of the total kinetic energy in the simulation, the filter width is well in the inertial subrange of the kinetic energy spectrum. The turbulence resolution can then be monitored by inspecting the ratio of unresolved kinetic energy to the total kinetic energy.
\[ M(x) = \frac{K_{RES}}{K_{RES}+K_{SGS}}, \quad K_{RES} = \frac{1}{2} \left\| \langle \mathbf{u}(x) \rangle - \langle \mathbf{u}(x) \rangle \right\|^2, \] (84)

where \( K_{RES} \) is the resolved portion of the turbulent kinetic energy (TKE), and \( K_{SGS} \) is the sgs kinetic energy.

**Figure 4.6** shows the measure of turbulence resolution \( M(x) \) defined by Eq. (84) for the simulations of nozzle B from Paper I. The left graph in **Figure 4.6** shows the turbulence resolution when using the Deardorff model, while the graph on the right shows the same metric when using the dynamic Smagorinsky model. For the dynamic Smagorinsky model, over 60% of the turbulent kinetic energy is resolved on all grid resolutions. With both models, a 1 cm grid is needed for the resolution metric to reach the “Pope criterion” of MTR<0.2.

The results in **Figure 4.6** agree with the prior analysis of Section 4.2.2. On the coarsest grid, the sgs model accounts for almost all of the TKE. Therefore, without the turbulent dispersion model, the droplets do not see the gas phase turbulence, leading to the weaker dispersion of particles from the jet centerline observed with the Deardorff model.

**Figure 4.6** Measure of turbulence resolution in the simulations of NFPA tests of micro nozzle B from Paper I. Left: Deardorff model Right: Dynamic Smagorinsky model.

Subramaniam [99] pointed out that, as usually implemented, LE methods are not convergent. Traditional LE methods use a fixed number of particles to describe the spray. When the grid is refined, the number of computational particles per grid cell decreases. As a result of this, the statistical error in estimated source terms in each grid cell increases. This may lead to a counter-intuitive result where the error in predictions increases as the grid is refined. Garg et al. [127] formulated a model for the error in interphase momentum transfer

\[ \epsilon = \frac{a}{N_p} + \frac{b(\delta x)}{N_p} + \frac{c}{\delta x^2}. \] (85)

The terms on the right-hand side represent statistical estimation error, bias error, and discretization error. Equation (85) highlights the dependence of the error in two-way coupling on both the grid size and the number of particles.
The large differences between the 0.5 cm and 1 cm grid shown by Figure 4.2 may be related to the above described estimation error. In the simulations discussed in section 4.2.2, the number of particles used to describe the spray was held constant for all grid resolutions. This would lead to increased stochastic error in estimating the two-way coupling terms and therefore possibly increasing the resolved turbulence. This increased turbulence in turn would have a reducing effect on the velocities and fluxes similar to the effect of using the dynamic Smagorinsky model.

It was found in Paper I that the grid resolution had a large effect on the simulation results. For multi-orifice spray heads, it is important that each of the individual orifices discharges within a different computational cell. This implies that the offset parameter and grid resolution need to be selected so that there are separate spray jets for each orifice. This is challenging to achieve if the perimeter angle of the spray nozzles is small. Furthermore, the number of Lagrangian particles used to describe the spray needs to be sufficiently high. The greater the number of particles used to describe the spray, the smoother is the predicted droplet density field.

4.3 Liquid pool fire modeling

4.3.1 Verification

A straightforward test for the liquid evaporation model is to see whether, given an imposed heat flux, the correct amount of liquid is evaporated. After the initial heat up phase, it is expected that the liquid will evaporate at a rate equal to \( \dot{q}'' = \dot{q}''/(\Delta h_g) \). Here \( \Delta h_g \) is the sensible enthalpy of evaporation, \( \Delta h_g = \Delta h_v + \int_{T_b}^{T_0} c_p dT \). To decrease the initial transients involved, the in-depth radiation transfer is ignored. Figure 4.7 shows the results of the mass conservation test. The model does not exactly conserve mass. This is possibly due to the remeshing procedure used in the condensed phase solver. Apart from the initial transient, the evaporation rate is relatively close to being correct. Note that errors in the prediction of the surface temperature in the simulation will cause the evaporation rate to differ from the theoretical value. Inaccuracy in calculating the mass transfer coefficient partly causes the difference in the evaporation rate. The surface temperature does not reach the boiling point of the liquid and the effective \( \Delta h_g \) value in the simulation will differ from the exact one.

Figure 4.7 also shows the evaporation rate of water in the ASTM flame spread apparatus and a mass conservation test of water evaporating under 50 kW/m² heat flux. While not strictly a verification test, it is simple enough to be used for checking the accuracy of the model implementation. The theoretical evaporation rate is within 3 % of the steady portion of the experimentally measured evaporation rate. The peak evaporation rate predicted by the evaporation model coincides with this value.
4.3.2 Validation of steady state burning rate predictions

In Paper IV and Paper V, the steady state burning rates of pool fires in open atmosphere and compartments were compared with experiments. Figure 4.8 shows a summary of the results for large pool fires in open atmosphere. In addition to experimental data, Figure 4.8 compares the predictions with the correlations [43,47]:

\[
\dot{m}_n = \frac{\dot{q}_n}{\Delta h_b}, \quad \dot{q}_n = 12.5 + 68.3 y_b^{1/4} \left(1 - \exp \left[ - \left( \frac{4}{3} \Delta h_b D \right)^{3/2} \right] \right). \quad (86)
\]

\[
\dot{m}_n = 0.001 \frac{\Delta h_v}{\Delta h_b} \Delta h_b \Delta h_v + \int_{T_b}^{T_a} c_v dT \quad (87)
\]

The simulation results follow the general trends in burning rates for large pool fires. Except for methanol and butane, the burning rates are over-predicted compared to experimental data. Grid resolution effects at least partly cause the over-prediction. Section 4.3.4 discusses these effects in more detail.
Figure 4.8 Comparison of predicted pool fire burning rates in open atmosphere with correlations and experimental measurements. Experimental data from Mudan [43], Klassen and Gore [128], and Ditch et al. [47]. The dashed line is Eq. (87) and the diamonds correspond to the correlation given by Eq. (86). Figure reproduced from Paper IV.

Paper V studied the effect of decreased oxygen concentration on the steady state burning rates of TPH pool fires. Figure 4.9 summarizes the results. The predicted burning rates are averaged over the steady state burning portion. The model predictions tend to be slightly higher than the experimental data. In one case, burning rate oscillations appeared in the simulations. In this case, the averaged burning rate is lower than in the experiments since the averaging is made over the oscillations. Figure 4.9 also shows the correlation [53]

$$\frac{\dot{m}_v}{\dot{m}_0} = 10X_{O_2} - 1.1,$$

where $\dot{m}_0$ is the burning rate of the pool fire in open atmosphere, and $X_{O_2}$ is the oxygen volume fraction near the pool base.
The appearance of burning rate oscillations in the compartment simulations is an apparent failure of the model. On the other hand, the result indicates that all the physics required to replicate the oscillations observed in other experiments [18] is included in the present FDS.

Overall, the steady state burning rates were predicted with accuracy similar to empirical correlations. Neither the 1-meter pool models nor the TPH pool models considered the effect of convection. This indicates that in-depth transport is likely to be important mostly in the initial heat up phase of the pool fire and possibly near the end. The next section discusses the effects of heat transfer within the liquid.

4.3.3 Effect of liquid side heat transfer

In Paper II, we tested the effects of in-depth absorption of radiation and heat transfer using data for water evaporation and an ethanol pool fire. Figure 4.10 presents results using two methods for determining the effective absorption coefficient (M1 and M2) and results from ignoring in-depth absorption of radiation (M3). Thermal conductivity was either the molecular value of thermal conductivity or the effective thermal conductivity defined in section 3.3.3. The thermal conductivity values are calculated with the corrected method of determining the effective thermal conductivity.
The mean absorption coefficient that produces the more realistic heat source distribution (M2) does not reproduce the gradually increasing heat release rate of the ethanol pool fire. The evaporation rate of water in the fire propagation apparatus is also steady. Method 1 (M1) produces slowly increasing evaporation rates in both cases. This method attempts to model the fraction of radiation passing through the liquid layer correctly. The lower absorption coefficient associated with Method M1 leads to radiation absorption deeper in the liquid.

Ignoring in-depth radiation (M3) absorption gives virtually identical results to method M2. This is likely a result of the relatively high value of absorption coefficient for ethanol. For radiation from ethanol flames, ethanol liquid is optically thick. The results could be different for other liquid fuels and thinner layers.

Liquid phase temperature data were not available for either experiment. Figure 4.11 shows profiles of liquid temperature in the water evaporation simulations. Liquid temperature is on the y-axis and height from the bottom of the pool on the x-axis. The models that produce gradually increasing burning rates in the ethanol pool fire case (M1K2 and M1K1) produced unphysical temperature distributions in the water evaporation case. The increasing temperature gradient near the liquid surface caused the increasing trend in burning rates seen in Figure 4.10. In a real pool fire, liquid convection could have a similar effect of changing the temperature gradient by transporting heat deeper into the liquid.
Figure 4.11 Predicted temperature profiles within the liquid in the simulation of water evaporation. Unphysical temperatures in the liquid phase in the water evaporation experiments.

In Paper IV, the predicted temperatures within a TPH pool are compared to the measured temperatures. Figure 4.12 displays the results from a simulation of a TPH fire in open atmosphere. The absorption coefficient was calculated using method M2 with data for DTE-medium oil because data for TPH was not available. The results show that the presently employed models are not capable of capturing the thermal gradient within the liquid. The heat penetration depth in the liquid is much thicker than is predicted by the model. The inaccuracy in the prediction of heat penetration is at least partly caused by the use of the absorption coefficient for DTE-Medium Oil.

Liquid temperatures in the simulation do not reach the specified boiling temperature. This is due to over-prediction of the mass transfer coefficient. Various stages in the burning rate of the pool fire can be matched with the development of the temperature gradient in the liquid. Up to around 300 seconds, the burning rate increases very gradually, as the surface slowly reaches boiling temperature.

Figure 4.12 Left: Burning rate of a TPH pool fire in open atmosphere. Right: temperatures within the liquid. Experimental data from the PRISME SOURCE S3 experiment.
The peak evaporation rates for the liquid evaporation and pool fire cases are close to the experimental values. The models are not able to reproduce the transient features of the evaporation rate. The simulations and the experimental data show that the transient features are related to the heat transfer within the liquid.

From the results, it seems apparent that the boundary layer resistance to mass transfer may only be significant when the liquid temperature is far from the boiling point. This is the case during the initial stages of pool fire burning and flame spread. Using a more accurate mass transfer model together with the one-dimensional, “transparent solid” - approximation is problematic. If the flame produces a very uneven radiative heat flux to the surface, a one-dimensional model will result in an uneven surface temperature and therefore an uneven burning rate. However, it seems improbable that significant differences in surface temperature could persist in a real pool fire. The uneven burning rate and heat flux would tend to mix the top layer of fuel, producing a uniform surface temperature.

**4.3.4 Grid resolution requirements**

The grid convergence tests in Paper II showed that for square heptane pool fires in open atmosphere and with 0.5 to 3-meter side length, the predicted burning rate on the coarsest grid was up to 40% higher than on the finest grid. However, full grid convergence could not be achieved in the burning rate prediction simulations.

In order to assess the role of the gas phase modeling in the grid dependence of burning rates, we carried out pool fire simulations with specified fuel mass flux. These cases were identical to the burning rate prediction simulations, except that the evaporation was specified, not predicted. The mass flux was calculated from the correlation [44]:

\[
\dot{m}^e = \dot{m}_\infty^e (1 - \exp(-k\beta D)).
\]

(89)
Figure 4.13 Convergence of incident heat flux as a function of grid size for different size burners.

For buoyancy dominated flows, such as flames from a pool fire, the grid resolution between two models can be compared using the Plume Resolution Index (RI) [129]. The RI is defined as

$$RI = \frac{D^*}{\delta x},$$

where $\delta x$ is the nominal size of a mesh cell, and $D^*$ is a characteristic fire diameter

$$D^* = \left[ \frac{\dot{Q}}{P_\infty c_p T_\infty \sqrt{g}} \right]^\frac{2}{5}.$$

Here $\dot{Q}$ is the total heat release rate of the fire. $D^*$ is related to the characteristic fire power $Q^*$ via the relation $Q^* = (D^*/D)^{5/2}$, where $D$ is the physical diameter of the fire. $D^*$ can be viewed as a measure of the integral length scale in the flame. The near wall grid resolution can be monitored in terms of $y^+$.

We measured the average incident heat flux to the burner surface at different grid resolutions and for various burner sizes. Figure 4.13 shows the results of the grid convergence study. The solid line corresponds to the expected incident heat flux $\dot{q}_{in} = m^*/\Delta h_g$. Incident heat flux predictions converge around $D^*/\delta x = 50$ for larger pool fires and at about $D^*/\delta x = 40$ for smaller pool fires. This is in line with experimental findings, in which the ratio of integral length scale to the pool size is found to get smaller as the pool size increases.

Grid convergence results in Paper IV showed that in compartment fire scenarios the burning rate predictions are less sensitive to the grid resolution. Since only a limited number of experiments with a single fuel were considered, no general conclusions can be made from this observation. However, the results from Paper II
and Paper IV suggest that the primary source of grid sensitivity of the burning rate predictions lies in predicting the radiative heat flux to the surface.

4.4 Risk analysis

4.4.1 Motivation

The stated goal of this thesis is to produce models for simulation of large scale incidents. Paper III presents an application of the methods developed in this thesis. The application part of Paper III studied the physical extent of the flames and smoke generated by the combustion of jet fuel from the impact of a commercial aircraft on an NPP reactor building. The goal was to investigate how far from the impact point the flames can reach to cause a possible threat to the components of the plant. In addition to the assessment of physical separation, the amount of fuel that does not burn in the initial fireball was recorded.

We conducted the risk analysis in two parts. The first part examined the effects of mean droplet size and impact height on the amount of accumulated fuel. After this, simulations of aircraft impact on a full-scale model of a nuclear island were conducted.

4.4.2 Validation of predicted fireball lifetimes and diameters

The threat posed by a fireball is proportional to its size, shape and lifetime. Therefore, for risk analysis purposes it is important that these aspects can be accurately predicted. Paper IV compared the predicted fireball lifetimes and diameters with empirical correlations. The relevant length and time scales of fireballs, based on dimensional analysis, are given by [77]:

\[ L_* = \left( \frac{MA_h}{\rho_0 c \rho_m c} \right)^{\frac{1}{3}} \quad U_* = \sqrt{L_* g} \quad \text{and} \quad t_* = \sqrt{L_* g}. \]  \( (92) \)

Here \( M \) is the fuel mass and \( \Delta h_c \) is the heat of combustion. Roper et. al. determined an experimental correlation for fireball lifetimes resulting from vertical fuel releases [79]. The correlation, stated in terms of the fireball length and timescales in Eq. (92), is:

\[ \frac{t_*}{t_{FB}} = 0.22 + 0.01Fr^2 \quad ; \quad Fr = \left( \frac{U_0}{U_*} \right)^2. \]  \( (93) \)

Numerical simulations were performed in a domain of \( 4L_* \times 4L_* \times 8L_* \), and fuel was inserted in the time interval \( t_{in} = [0,0.1t_{FB}] \). The domain was discretized with 220 \times 220 \times 550 cells. The droplet size distribution was based on liquid missile impact experiments. However, very large droplets were observed to rain out of the fireball before they evaporate. Therefore the width parameter was increased to decrease the number of very large droplets. The fuel insertion was modeled as a
A vertical fuel spray with a spray angle of 15°. Nine simulations were performed with fuel masses of 10, 1000, or 10,000 kg and initial velocities of 50, 200, or 300 m/s.

We defined the end of the fireball lifetime as the time at which 95% of the fuel is burned. The start of the fireball lifetime was taken as 0.5\(t_{in}\). This definition of the start of the fireball lifetime was also used by Roper et al. They defined the end of the fireball lifetime as the time when flames were no longer visible.

Figure 4.14 compares the simulation results with Eq. (92). Overall, the simulated results showed good agreement with the correlation. The predicted fireball lifetimes were within 15% of the values predicted by Eq. (92). Despite the low-Mach number limitation of FDS, there were no significant deviations from the general trend, even for cases in which the droplets were inserted at 300 m/s.

![Figure 4.14 Comparison of predicted Fireball lifetimes with correlation.](image)

Figure 4.14 Comparison of predicted Fireball lifetimes with correlation.

Figure 4.15 shows the contours of the gas temperature at the midplane of a fireball. The contours are shown at time instants \(t_{FB} = 0.3, 0.6,\) and 0.9 and for an initial velocity \(V_0 = 200\) m/s. The top of Figure 4.15 shows the results for the case with \(M = 10,000\) kg, and the bottom shows the results for the case with \(M = 10\) kg. At the early stages of the fireball development, the hot gas cloud was still shaped like a jet. At about halfway through its lifetime, the fuel jet decelerated, and its movement was now controlled by buoyancy. In the final stages, the cloud rolled up in a vortex, reaching its final size. The vortex roll up started earlier for the \(M = 10,000\) kg case owing to the lower Froude number. If the 1000 °C contour is taken as the fireball edge, the maximum fireball diameter can be visually approximated from Figure 4.15 to be \(\sim 1.2L_e\). This falls within the range given by correlations for fireball diameter.

The threat posed by a fireball is related to the dose of thermal radiation absorbed by the target under investigation. The thermal radiation dose is determined by the duration and diameter of the fireball. The results from Paper III, summarized in this
section, show that FDS can predict these parameters within 20 % of experimental correlations.

Figure 4.15 Instantaneous temperature contours for fireballs with $U_{ini} = 200$ m/s at time instants $t/t_{FB} = 0.3, 0.6, 0.9$. Top: $M = 10,000$ kg. Bottom: $M = 10$ kg
4.4.3 The effect of impact height and droplet size on pooling fraction

An important aspect of the fires resulting from an aircraft impact is the fraction of the fuel that does not burn in the initial fireball. We call this quantity “the pooling fraction”. The specific amount of remaining fuel depends on both the droplet size and impact height. The closer the impact location is to the ground, the larger the pooling fraction. Because smaller droplets evaporate faster than larger droplets, a lower average droplet diameter results in smaller pooling fractions. Paper III presents a sensitivity study considering the relationship between impact height and pooling fraction.

![Simulation domain used for the pooling fraction sensitivity analysis.](image)

Some numerical experiments were carried out to quantify the effect of impact height and droplet size on the pooling fraction. The simulation domain consisted of a rectangular building 40 meters wide and 50 meters high. The impact location on the building was varied. **Figure 4.17** illustrates the simulation model and impact locations. 10 000 kg of fuel was released in 0.1 seconds. Grid resolution was 1.0 meter.
Figure 4.17 Sensitivity of pooling fraction to droplet size and to impact height.

The bottom graph in Figure 4.17 shows the pooling fraction as a function of the impact height for the droplet distribution with $d_{50} = 80 \mu m$. As the impact location moves closer to the ground, the fraction of fuel left unburnt increases significantly. At a height of 5 m, the pooling fraction is almost 30%. For impact heights above 20 m, the pooling fraction is practically zero.

The median volumetric diameter has a more modest effect (see the top graph in Figure 4.17). For an impact height of 10 m, the pooling fraction varies between 11 % and 18 % for median diameters in the range of 40 \( \mu m \) to 180 \( \mu m \). The growth of the pooling fraction tapers off at just below 20%.

Two conclusions can be made from these results. The first is that with realistic droplet size distributions a significant fraction of the fuel ejected from a plane may accumulate in pools. The second conclusion is that the pooling fraction is more sensitive to the geometry surrounding the impact location than to the droplet size.
When the impact location is closer to the ground, the liquid jets do not have time to evaporate before impact.

### 4.4.4 Simulation of a plane impact on a nuclear island

The simulation model of the NPP included the reactor building (cylindrical shape with a diameter of 56 m), four auxiliary buildings attached to the reactor building, part of the diesel building, and part of the turbine hall (details of the model can be found in Paper III).

The impact scenario was the horizontal impact of a commercial aircraft, carrying 10 tons of fuel, at a speed of 125 m/s in the direction normal to the reactor building wall. The impact height was 35 m from the ground and approximately 10 m from the roof of the auxiliary building. Five different impact positions were considered, and the effect of wind was investigated by assuming either 10m/s wind speed or no wind (See Figure 4.18). Eight possible wind directions were considered.

![Figure 4.18 Impact locations and monitoring points used in the simulation of plane impact on a nuclear island.](image)

Gas temperature, gas velocity, and fuel gas volume fraction were monitored at six locations denoted A–F. The maximum observed value of each monitored quantity over the entire simulation was recorded for each measurement location. This observed value was then used to indicate whether the conditions at the measurement point can be considered hazardous. Figure 4.18 shows an overview of the simulation model and the monitoring locations.

In the analysis of the simulations, we treated the impact location and wind direction and measurement location as random variables. This allowed us to derive probability density functions for seeing threatening conditions in a randomly selected spot on the main building. The placement of the monitoring locations A–D around the dome also allowed us to determine the sufficiency of physical separation.

The simulation results showed that direct contact with the flame was limited to a region of the building complex that covered less than half of the reactor building perimeter. Flames lasting longer than about one second were observed in a sector that reached 45° - 90° in both directions from the direction of the incoming aircraft.
The probability of any individual target at the height of the roofs of the auxiliary buildings and close to the reactor building becoming engulfed by flames was between 25% and 50%. For objects placed at two opposite sides of the reactor building, physical separation was realized. Figure 4.19 illustrates the conclusions drawn from the simulations.

In addition to the gas phase quantities, we also investigated the amount of fuel deposited on the reactor building. In the majority of the simulations, the amount of accumulated fuel was between 10 and 30% of the total amount. In 40% of the simulated scenarios, the amount of fuel burning on the surfaces was more than 20%. The fuel accumulated on the roof near the impact location and also on the reactor dome.

Figure 4.19 Possible and likely regions of aircraft impact flame contact around the NPP reactor building in the case of a horizontal impact at a height of 35 m and releasing 10 t of fuel.
5. Conclusions

Papers I-V present modeling and validation of three fire-related phenomena: liquid transport in a spray, rapid spray combustion, and liquid pool burning. Paper I deals with water sprays formed by high-pressure water mist nozzles. Papers II and III discuss liquid sprays from missile impacts. Despite the apparent differences in the formation mechanisms of the sprays, the droplet sizes and speeds were relatively similar. Both types of sprays can be simulated using the LE method, when the spray boundary condition is correctly defined.

The correct prediction of air entrainment into liquid sprays is crucial for successful predictions of spray penetration and dispersion. The correct amount of air entrainment is predicted if the spray boundary condition is defined appropriately.

Firstly, the droplets need to have the correct initial velocity. In this work, the initial velocity of the droplets accounted for all of the momentum of the injected liquid. This ensures that the correct amount of momentum is inserted. Modifying initial velocity of the gas phase at the spray boundary condition was not necessary.

Secondly, the droplet size distribution can be selected to represent a stable size further away from the nozzle. In fact, any other choice would necessitate the use of secondary breakup models.

In Paper III, we applied the developed models to simulations of airplane impact on a nuclear island. Based on the results of these simulations we made the following conclusions:

1. The simulated fireballs resulted in locally high temperatures and velocities but only for a short duration. Physical separation was realized for targets situated on opposite sides of the building.
2. Droplet size and the geometry surrounding the impact location have a significant effect on the pooling fraction. Lower impact location and larger average droplet size lead to larger pooling fractions.
3. Up to 20% of the fuel involved in the crash accumulated on the surfaces of the target building. The subsequent burning of this fuel may then be a significant hazard to the safety of the NPP and should not be ignored. The pool fire models developed in this thesis could be directly applied to predict the consequences of the resulting pool fires.

Papers IV and V showed that the steady state burning rates in compartments and open atmosphere could be predicted with accuracy similar to empirical correlations.

The grid resolution requirements for accurate burning rate predictions of open pool fires are very demanding. Accurate steady state burning rates could be predicted in compartment fire scenarios on relatively coarse grids. Together, these results suggest that the key to easing the grid resolution requirements lies in the modeling of the radiation transport.

Paper IV showed that the in-depth heat transfer, in the form of the in-depth radiation absorption and enhanced heat transfer in the liquid due to convective motions, might be important in predicting the detailed dynamics of the fire. However,
the models employed are not capable of accounting for all the phenomena in the liquid. The gray gas approximation of the radiation transport cannot correctly predict the transport of radiation through the liquids. This prediction could be improved by resolving the wavelength dependence of absorption and re-radiation. In the current model, heat transfer is one dimensional. In real liquids, the heat transfer by convection in the lateral direction could play a significant role. Better models for the internal heat transfer may be needed to capture the dynamics of pool fires correctly. A better evaporation model may also be needed in conjunction with the improved heat transfer models.
6. Future work

The results presented in this thesis support the conviction of previous researchers that radiation modeling is the key factor in predicting burning rates in CFD simulations. One avenue that should be explored is spectrally resolved solutions of the radiative transfer equations. This would be required for prediction of both the heat feedback to the fuel surface and the radiation heat transfer within the liquid. For a liquid layer a few millimeters thick, a significant portion of the incident radiation will pass through the layer. In such cases, the modeling of in-depth radiation transport and heat transfer to the substrate is likely to be the key in predicting the burning rate.

The mass transfer resistance to evaporation is relatively unimportant for predicting the steady state burning rates of deep pools, but could have a significant effect in cases in which it is attempted to predict the formation of flammable clouds from liquid spills. A better model based on e.g. wall functions could help in this respect. Better experimental data is needed for liquid evaporation from surfaces under relevant conditions.

There are still several open questions concerning the heat transfer mechanisms in pool fires. It would be interesting to see the results of studies in which full 3D predictions of heat transfer through the pan and within the liquid were coupled with gas phase solution. Such simulations could offer insight into the mechanisms of lip height effects and radiation absorption within the fuel.

The characterization of the initial spray is still an open research question. Highly resolved measurements near the spray inlet would be required to validate the Gaussian profile assumption made in section 3.2.3.

The grid resolution requirements of predictive pool fires and spray simulations are still prohibitive for everyday engineering use. The effect of the subgrid scales on particle motion is likely to be important, considering the coarse resolutions used in engineering calculations of suppression systems. Turbulent dispersion models such as the one discussed in this work could be pursued.

The number of computational droplets used to describe the spray may also be a limiting factor in engineering applications. Droplet density control algorithms could be explored to alleviate these problems.
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