



Modeling the Impact of Kerosene Droplet Distributions Using the Rosin-Rammler Method in HVOF Thermal Spray via CFD

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نمذجة تأثير توزيع قطرات الكيروسين باستخدام طريقة روزين-رامملر في الرش الحراري HVOF عبر ديناميكا الموائع الحسابية

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Abstract

This study numerically investigates the influence of droplet size distribution on the kerosene flame characteristics relevant to thermal spray processes, using the ANSYS Fluent solver coupled with (SST) k- ω turbulence, EDM combustion, and P-1 radiation models. We simulated droplet behavior using the Lagrangian Discrete Phase Model (DPM). We compared nine distinct size distributions: six utilizing the Rosin-Rammler (R-R) distribution (varying Mean Diameter $\bar{d}$ and Spread Parameter n) against three Uniform Distributions as a baseline. The simulation results exhibited strong agreement with experimental and published thermal data primarily for the finer R-R distributions (Cases 1 and 2). This superior performance is consistent with the literature indicating that kerosene droplets $\leq 3 \mu\text{m}$ transition almost entirely to the vapor phase immediately upon injection. Analysis indicated that ($\bar{d}$) is the dominant factor: smaller ($\bar{d}$) led to rapid vaporization and confined high-temperature zones, while larger ($\bar{d}$) delayed combustion, leading to flame extension outside the chamber. Furthermore, the polydisperse R-R sprays resulted in a more stable flame structure compared to the Uniform cases, which produced localized evaporation and excessively sharp thermal gradients. These findings underscore the necessity of accurately modeling the inherent size variability of atomized fuel for optimizing thermal spray flame efficiency and confinement.



Keywords: Rosin-Rammler Distribution, Thermal Spray, Kerosene Combustion, Droplet Dynamics, CFD Simulation.

المخلص

تبحث هذه الدراسة عددًا في تأثير توزيع أحجام القطرات على خصائص لهب الكيروسين ذات الصلة بعمليات الرش الحراري، باستخدام برنامج ANSYS Fluent مقتربًا بنموذج الاضطراب $k-\omega$ (SST)، ونموذج الاحتراق EDM، ونموذج الإشعاع P-1. تم تمثيل سلوك القطرات باستخدام نموذج الطور المنفصل (DPM) بطريقة لاغرانج. تمت مقارنة تسع توزيعات مختلفة لأحجام القطرات: ستة منها باستخدام توزيع روزين-راملر (Rosin-Rammler) مع تغيير كل من القطر المتوسط ($\bar{d}$) ومعامل الانتشار n وثلاثة توزيعات منتظمة (Uniform) استخدمت كحالة مرجعية أظهرت نتائج المحاكاة توافقًا قويًا مع البيانات الحرارية التجريبية والمنشورة، خاصة في الحالات ذات التوزيعات الدقيقة من نوع روزين-راملر (الحالتان 1 و 2). ويتمشى هذا الأداء المتفوق مع ما ورد في الأدبيات التي تشير إلى أن قطرات الكيروسين التي يبلغ قطرها ≥ 3 ميكرومتر تتحول تقريبًا بالكامل إلى الطور البخاري فور حقنها. أظهر التحليل أن القطر المتوسط ($\bar{d}$) هو العامل الرئيسي: إذ يؤدي صغر ($\bar{d}$) إلى تبخر سريع وتكون مناطق ذات درجات حرارة مرتفعة ومحصورة، بينما يؤدي كبر ($\bar{d}$) إلى احتراق متأخر وامتداد اللهب خارج غرفة الاحتراق. علاوة على ذلك، أظهرت الرشّات متعددة الأحجام وفق توزيع روزين-راملر لها أكثر استقرارًا مقارنةً بالحالات المنتظمة، التي نتج عنها تبخر موضعي وتدرجات حرارية حادة بشكل مفرط. تؤكد هذه النتائج على ضرورة النمذجة الدقيقة للتنوع الطبيعي في أحجام القطرات الناتجة عن عملية التذرية (الأتمة) للوقود، من أجل تحسين كفاءة اللهب في عمليات الرش الحراري وضمان انحصاره داخل الغرفة.

الكلمات الدالة: توزيع روزين-راملر، الرش الحراري، احتراق الكيروسين، ديناميكيات القطرات، المحاكاة الديناميكية للموائع الحسابية (CFD).

1. Introduction

Thermal spraying is a cornerstone of surface engineering, offering scalable solutions to enhance material durability against wear, corrosion, and thermal degradation in demanding environments (Pawlowski, 2008). By applying coatings such as metals, ceramics, or composites, this technology significantly extends the operational lifespan of critical components in industries ranging from aerospace to biomedical engineering (Davis, 2004). The process involves heating or melting feedstock materials like powders or wires and propelling them at high velocities onto a substrate, where they form dense, adherent layers (Fauchais et al., 2014). One of the most advanced thermal spraying methods is High-Velocity Oxy-Fuel (HVOF) spraying. Introduced in the 1980s, HVOF combines combustion energy with supersonic gas dynamics to produce high-energy jets that deposit coatings with exceptional bond strength, low porosity, and high density (Krey et al., 1996; Tan et al.,



2018). This makes it particularly valuable for applications requiring resistance to extreme thermal and mechanical stresses, such as turbine blades in aerospace or wear-resistant coatings for energy sector components (Padture et al., 2002; Niemi et al., 1991). Despite its advantages, optimizing the HVOF process remains a challenge. Key factors such as combustion dynamics, gas-particle interactions, and substrate cooling create a system sensitive to minor variations in operational conditions (Kamnis & Gu, 2006). Among these, the size distribution of kerosene droplets during atomization is a critical factor that has yet to be fully explored. Variations in droplet size can result in incomplete combustion, uneven heat distribution, and poor particle heating, negatively affecting coating quality (Tabbara & Gu, 2009; Picas et al., 2013).

Existing Computational Fluid Dynamics (CFD) models often simplify the process by assuming idealized droplet distributions, reducing their predictive accuracy in real-world applications (Bussmann et al., 2000; Ahmed & Hadfield, 2002). This has limited the effectiveness of simulations, especially in industrial settings that require precise control over coating properties. Additionally, experimental studies on the effects of droplet size are limited, and optimizing kerosene atomization remains largely empirical, relying on costly trial-and-error adjustments (Guessasma et al., 2004).

The chemical engineer plays a crucial role in advancing thermal coating techniques, particularly by investigating gas-particle interactions and improving combustion efficiency. Chemical engineers contribute to enhancing coating performance by optimizing key parameters such as droplet size distribution during kerosene atomization, ultimately improving the overall efficiency and quality of the thermal spraying process. Additionally, chemical engineers design feedstock materials used in the process and develop innovative techniques to improve energy efficiency and reduce waste in industrial applications (Kamnis & Gu, 2006; Guessasma et al., 2004).



Recently, (Kannan et al., 2023) employed a full 3D CFD approach to simulate not only the kerosene-oxygen gas dynamics, but also the in-flight behavior of solid particles such as CoNiCrAlY. Their work provided a validated framework for predicting particle velocity, temperature, and deposition profiles. Further, it highlighted the importance of stand-off distance and particle–substrate interaction in determining coating quality. Although this study introduced more realistic boundary conditions and included solid particle tracking, the liquid fuel droplets were still assumed to be of a single, uniform diameter, thereby overlooking the effects of droplet size distribution on combustion performance.

In this study, we aim to investigate the effect of using droplets with non-uniform size distributions. Specifically, a Rosin-Rammler distribution will be implemented to more accurately represent the droplet size spectrum generated by practical atomization processes, allowing for a more realistic simulation of combustion behavior and its influence on coating formation.

2. Methodology

2.1. Simulation Model Overview

The computational fluid dynamics (CFD) analysis was performed using ANSYS Fluent (v.23). This study focused specifically on simulating the atomization and kerosene combustion processes within the flame spray environment. Particle-related phenomena such as melting, trajectory after impact, and final deposition of solidified particles were intentionally excluded to isolate the effects of the combustion and droplet dynamics. The validity of the established simulation methodology was confirmed by comparing the model's calculated results (primarily focusing on thermal and flow fields) against experimental data provided in the published literature by Kannan et al. (2023). This approach ensures the fidelity of the baseline combustion and fluid dynamic setup before introducing the variable droplet distribution parameters.



2.2. Computational Domain and Meshing

The thermal spray process was modeled using a 2-D axisymmetric geometry to accurately represent the burner setup, which included the precursor injection point, dispersion gas inlets, pilot flame, and ambient environment. The domain was established to capture the region extending from the nozzle exit to the substrate location to account for the full development of the flame and particle behavior (Figure 1).

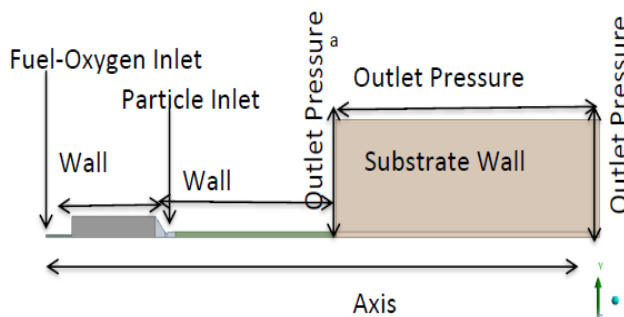


Figure 1. The computational domain in this work.

2.2.1. Geometry and Boundary Conditions:

The geometry incorporated all relevant injection and boundary points:

- Particle Inlet: Surface injection for precursor droplets through the capillary nozzle.
- Fuel-Oxygen Inlet: Mass flow inlets for dispersion oxygen and fuel.
- Ambient Boundaries: Pressure inlet/outlet boundaries for the ambient environment.
- Wall Boundaries: Walls for the nozzle, burner, and substrate, applying a no-slip condition.

2.2.2. Mesh Generation and Independence:

An initial structured quadrilateral mesh was generated (Figure 2). The mesh was progressively refined, specifically in the regions surrounding the nozzle and the flame zone, where steep gradients in velocity and temperature were anticipated.

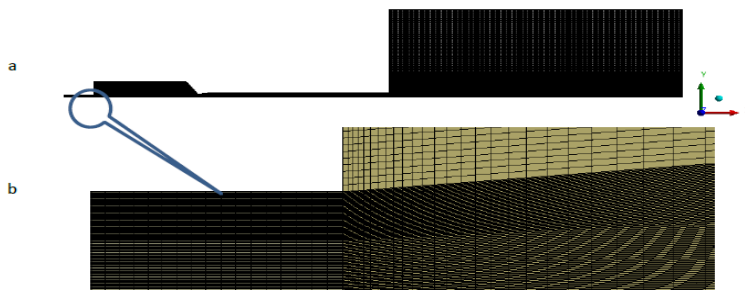


Figure 2. a) Initial mesh of the computational domain. b) Inset: refined mesh of the atomizer.

A mesh independence study was conducted using five different mesh sizes (ranging from 139,833 to 436,109 nodes) to ensure the independence of the grid resolution (Table 1). Mesh quality metrics, such as orthogonal quality (>0.1) and skewness (<0.8), were maintained according to standard CFD best practices.

Table 1. Quality parameters of different mesh sizes in this study.

Quality parameters	Initial mesh	Second mesh	Third mesh	Fourth mesh	Fifth mesh
Orthogonal quality should be >0.1	0.52683	0.53344	0.54044	0.54722	0.55248
Skewness should be <0.8	0.59621	0.59621	0.59621	0.59621	0.59621
Grid size, nodes	139833	185869	238703	330026	436109

The final mesh of approximately 330,026 nodes was selected as it yielded consistent centerline temperature predictions (Figure 3), providing an optimal balance between computational cost and accuracy.

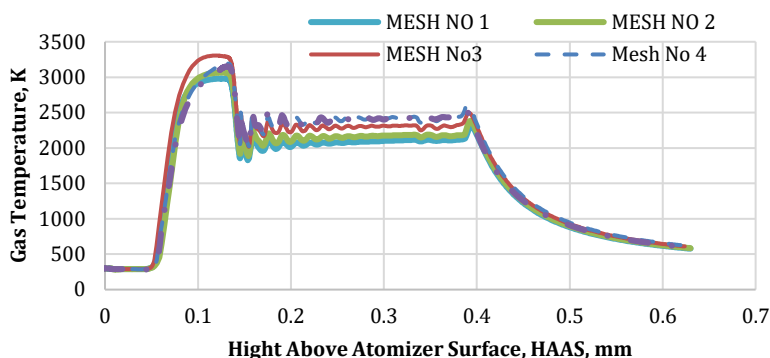


Figure 3. Centerline Temperature for 5 Different Mesh Sizes.

2.3. Physical Models and Governing Equations

The established geometric and meshing setup was implemented in ANSYS Fluent v.23 Ansys (2011). The following key physical models were employed and kept constant across all simulations:

2.3.1. Flow Solver and Turbulence:

A pressure-based solver was utilized alongside the (SST) k-omega turbulence model. This specific turbulence model was chosen due to its proven suitability for modeling axisymmetric, high-velocity jet flows characteristic of flame spray processes.

2.3.2. Combustion and Radiation Modeling:

To accurately capture the energy transfer and reaction kinetics, two additional models were integrated: The P-1 radiation model and the Eddy Dissipation Model (EDM) for combustion modeling.

2.4. Discrete Phase Model (DPM) and Rosin-Rammler (R-R) (The Core Variable)

2.4.1. Lagrangian Framework and Auxiliary Models:

Droplet behavior was simulated using the Lagrangian Discrete Phase Model (DPM) in ANSYS Fluent, tracking individual particle motion, heat transfer, and phase change. The governing equations for droplet motion and energy transfer were applied. The analysis incorporated forces including drag calculated via the Morsi and Alexander



correlation (Morsi & Alexander, 1972) and gravity. Additional phenomena such as droplet evaporation and stochastic turbulent dispersion were included using the Discrete Random Walk (DRW) model (Hutchinson et al., 1971; Kallio & Reeks, 1989) and the Eddy Interaction Model (EIM). A surface injection strategy was utilized to define droplet release location and initial velocity based on flow rate, and ideal gas assumptions were applied.

2.4.2. Rosin-Rammler (R-R) Case Studies Design:

This study employs a total of nine distinct case studies (Cases 1–9) to systematically analyze the influence of the droplet size spectrum on the kerosene combustion process. These cases are categorized into two main groups:

The first group is Rosin-Rammler Distribution (Cases 1–6): Six cases utilize the Rosin-Rammler (R-R) distribution, where the primary variables are the Mean Diameter ($\bar{d}$) and the Spread Parameter (n).

The second group is Uniform Distribution (Cases 7–9): Three cases utilize a Uniform Distribution (single diameter input) to serve as a baseline, with the diameter fixed to equivalent Mean Diameter values used in the R-R cases (e.g., Uniform Diameter 7 micron corresponds to an R-R case where ($\bar{d}$) = 7 micron).

The calculation methodology involves determining the Rosin-Rammler (R-R) parameters by fitting the size data. This calculation procedure is consistently applied to all six Rosin-Rammler case studies. The subsequent section will detail the Calculation Methodology for one specific case (Case 1 Example). The R-R distribution parameters are defined by two key parameters: the Mean Diameter ($\bar{d}$) and the Spread Parameter (n). These parameters, which dictate the shape of the droplet size spectrum, are the primary variables investigated in this study. Their values are typically derived by fitting cumulative mass fraction data (Y_d) to the R-R equation as following:

$$Y_d = \exp\left[-\left(\frac{d}{\bar{d}}\right)^n\right] \quad \text{..... (1)}$$



where;

Y_d is the cumulative mass fraction; this is the output of the equation. It represents the fraction (or percentage, if multiplied by 100) of the total mass (or volume) of droplets that have a diameter greater than the specific size $\bar{d}$ is always between 0 and 1.

d is the droplet (or Particle) diameter; this is the independent variable (the input size). It is the specific diameter you choose to define the fraction.

$\bar{d}$ is the mean diameter; this is one of the two key parameters that define the R-R curve. It is the size for which (Y_d) equals 1, or approximately 0.368 (36.8%). It defines the location or central tendency of the distribution.

n is the spread parameter (or Uniformity Index), this is the second key parameter that defines the R-R curve. It determines the width or uniformity of the size distribution. A larger n means a narrower (more uniform) range of droplet sizes, while a smaller n means a wider (more spread out) range.

A set of distinct case studies was created by systematically varying the values of $\bar{d}$ and n . For instance, the calculation methodology involves determining the $\bar{d}$ as the diameter at which the cumulative mass fraction is approximately ($0.368e^{-1}$). For the initial benchmark case (Case 1), the following R-R parameters were derived and implemented in ANSYS Fluent: The Mean Diameter ($\bar{d}$) was 4 microns, the Spread Parameter (n) was 1.1, the Minimum Diameter was 1 micron, and the Maximum Diameter was 50 microns.

To illustrate the parameter determination, Figure (4) shows the graphical relationship between the cumulative mass fraction (Y_d) and the diameter (d). The Mean Diameter ($\bar{d}$) is extracted from this curve at the point where the cumulative mass fraction greater than ($\bar{d}$) is approximately 0.368, as highlighted in the figure. These determined values are then used as the inputs for the DPM model in ANSYS Fluent for each case study.

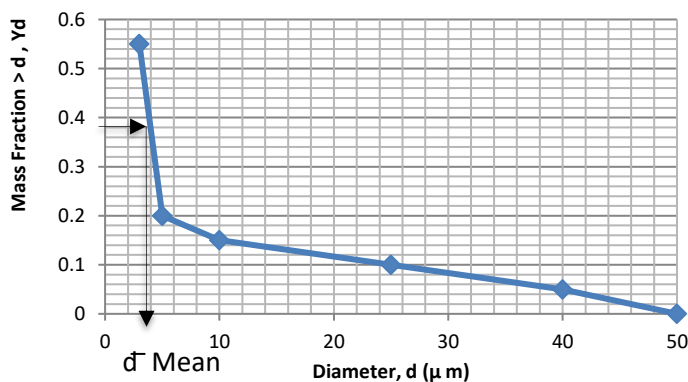


Figure 4. Rosin-Rammler Distribution Plot.

These determined values are then used as the inputs for the DPM model in ANSYS Fluent. The full set of parameters for all nine case studies is presented in Table (2).

Table 2. Fuel Droplet Distribution Parameters Used in CFD Studies
(Rosin-Rammler and Uniform Distribution).

Case Number	Distribution Type	Mean Diameter, d^- (μm)	Spread Parameter (n)	Initial Diameter (Uniform) (μm)
1	(RR) Narrower Distribution	2.5	0.54	NA
2	(RR)	3.5	1.23	NA
3	(RR)	7	0.53	NA
4	(RR) More Broadly Distributed	18	0.59	NA
5	(RR)	27	0.99	NA
6	(RR)	32	1.3	NA
7	Uniform Distribution	NA	NA	2.5
8	Uniform Distribution	NA	NA	7
9	Uniform Distribution	NA	NA	27



2.5. Numerical Scheme and Convergence

2.5.1. Numerical Scheme:

The governing equations were numerically solved using the Finite Volume Method (FVM) with a pressure-based solver in ANSYS Fluent. Pressure-velocity coupling was efficiently handled through the Coupled (COUPLED) algorithm. To ensure high accuracy and stability, a second-order upwind discretization scheme was adopted for all primary conservation equations (mass, momentum, energy, species, turbulence).

2.5.2. Initial Conditions and Phase Formulation:

The simulation domain was modeled as two distinct phases: the continuous phase (fuel, oxidizer, combustion products) described using the Eulerian framework with a two-dimensional Cartesian tensor formulation, and the discrete phase (liquid droplets) described using the Lagrangian DPM. Two-way coupling was enabled between these phases to account for momentum, mass, and energy exchanges under steady-state conditions. Initial conditions for all dependent variables (velocity, pressure, temperature, species concentrations) were specified to accelerate the solution stabilization and convergence rate.

2.6. Combustion and Droplet Dynamics Models

The following fixed physical models were utilized across all case studies:

- Instead of **assuming a fixed and uniform initial droplet diameter**, kerosene droplet size data (ranging from **1 to 50 microns**) reported in experimental literature were adopted and incorporated via the **Rosin-Rammler distribution method** (detailed in Section 2.4.2).
- Combustion Model: The Eddy Dissipation Model (EDM) was used to model combustion kinetics, treating the Kerosene-oxygen reaction as a single-step global mechanism.
- Radiative Heat Transfer: The P-1 radiation model was employed to capture radiative heat exchange between phases.



- Droplet Forces & Dispersion: Drag (Morsi and Alexander correlation) and gravity were incorporated. Heat and mass exchange (droplet evaporation) and stochastic turbulent dispersion were modeled using the Discrete Random Walk (DRW) model and the Eddy Interaction Model (EIM). A surface injection strategy was used to define initial droplet conditions based on flow rate and nozzle geometry.

2.7. Verification of Numerical Convergence

Numerical convergence was strictly verified by ensuring the reduction of normalized residuals below 10^{-4} for the continuity, momentum, and energy equations. This strict criterion confirms that the model achieved a steady-state condition with the required level of numerical accuracy.

3. Results and Discussion

3.1. Model Validation and Baseline Comparison

This section aims to validate the foundational simulation model by comparing the calculated results against reliable experimental data available in the literature. The validation was performed using measured radial temperature distribution data at the burner exit, sourced from the reference (Kannan et al., 2023). This region is of critical importance as it defines the initial conditions governing kerosene evaporation rates and ignition.

Figure 5 illustrates this comparison, presenting the simulated radial gas temperature distribution calculated for all six investigated case studies (using different Rosin-Rammler distributions) against the experimentally measured values taken from the reference. The comparison focused on the radial temperature distribution at the spray gun outlet. As shown in Figure (5), the simulated temperature profile closely matches the experimental data for Cases 1 and 2, with an average error of 6% across the evaluated positions. This strong agreement indicates that the model successfully captures core physical phenomena, including



combustion, atomization, and heat transfer. Minor differences observed near the barrel wall may result from measurement uncertainties or assumptions within the turbulence model.

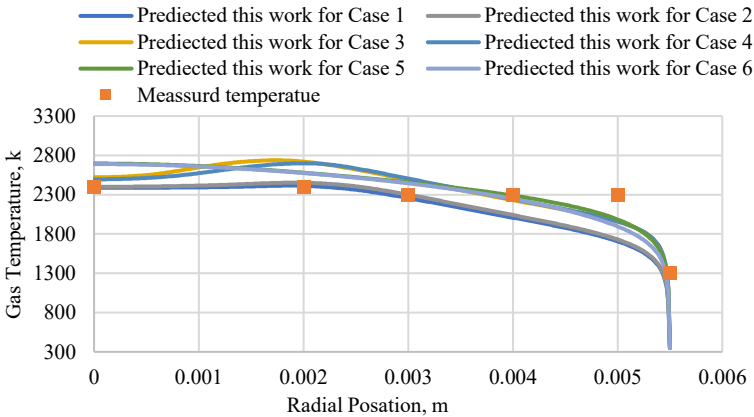


Figure 5. Comparison between predicted temperatures in this work and measured temperatures reported by Kannan et al. (2023).

3.2. Effect of Rosin-Rammler Parameters on Flame Structure

The influence of the Mean Diameter ($\bar{d}$) and the Spread Parameter (n) on the kerosene flame structure is analyzed through droplet size distributions (Figure 6) and gas temperature contours (Figure 7).

The thermal results show a direct link between the droplet size spectrum and the spatial location of the heat release; cases with smaller mean droplet diameters and narrower distributions (e.g., Cases 1 and 3) showed more complete combustion within the chamber. The rapid evaporation and burning of smaller droplets facilitated faster heat release, enabling fuel to burn internally (Figure 7).

In contrast, broader distributions with larger droplets (e.g., Cases 5 and 6) delayed combustion due to slower evaporation, causing part of the fuel to burn beyond the combustion chamber (Figure 8), which could compromise safety and efficiency.

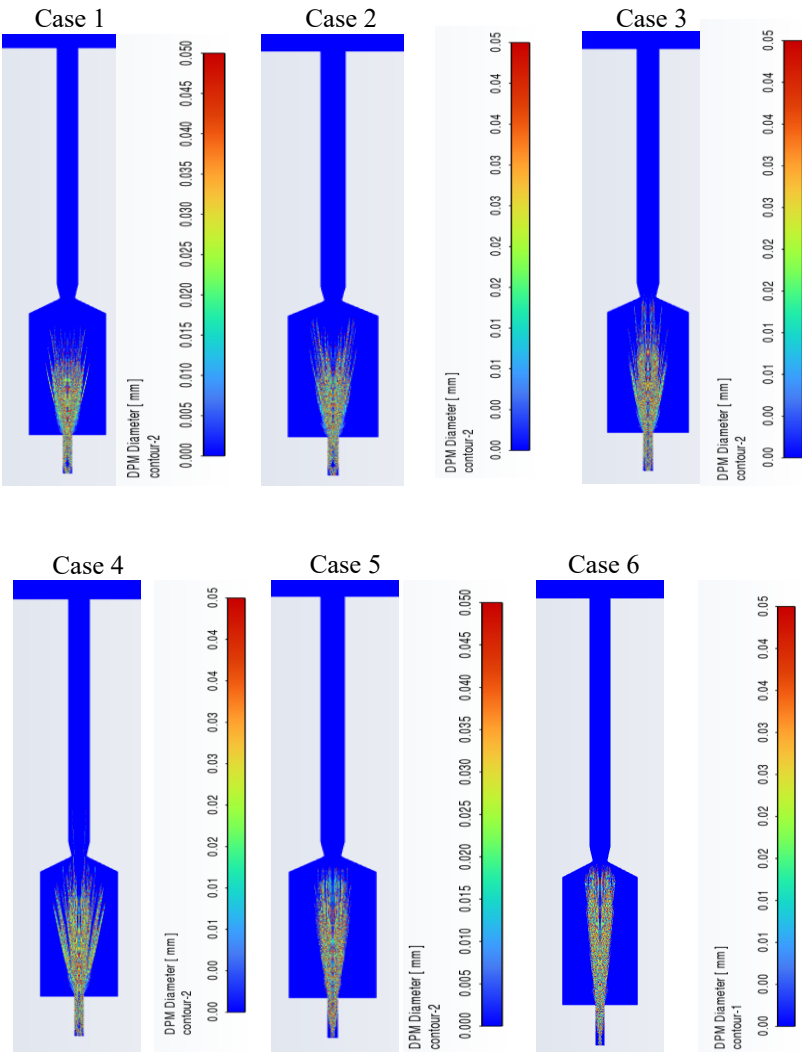


Figure 6. Droplet size distribution contours for cases 1 to 6.

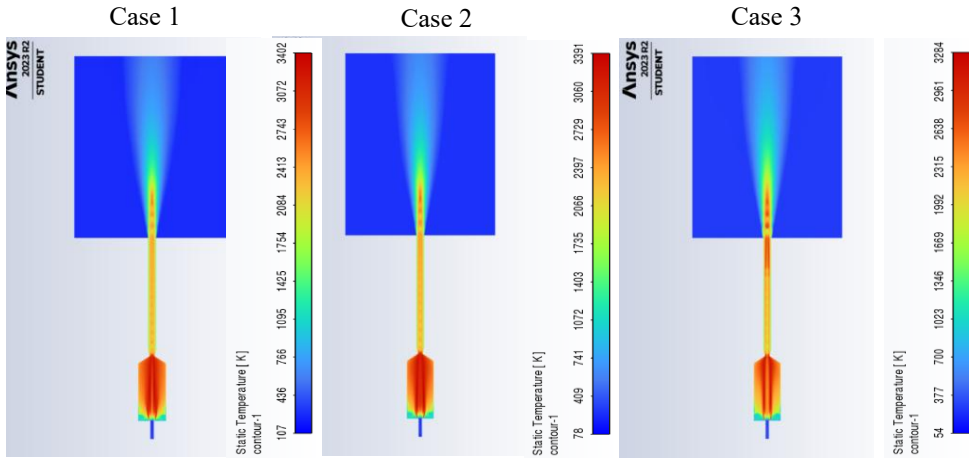


Figure 7. Gas temperature contours for Cases 1–3.

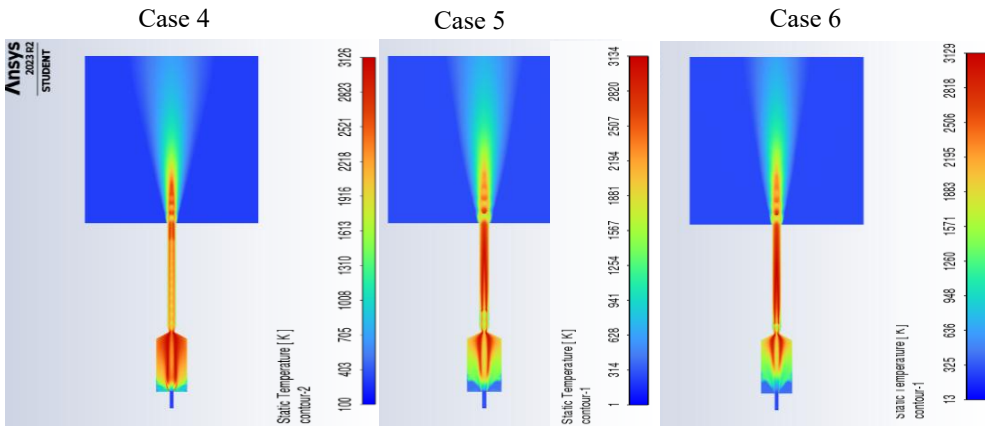


Figure 8. Gas temperature contours for Cases 4–6.

Simulated temperatures agreed well with measured values only in Cases 1 and 2. For other cases, higher simulated temperatures may reflect incomplete combustion or flame extension. These results highlight the importance of droplet size distribution in shaping thermal spray flame characteristics, influencing combustion location and efficiency.

3.5. Comparison with Uniform Droplet Size Injection

Cases 7, 8, and 9 used uniform droplet sizes matching the mean diameter of Cases 1, 3, and 5, respectively. Figure (9) shows these monodisperse cases lack the droplet

size variability present in the RR distribution.

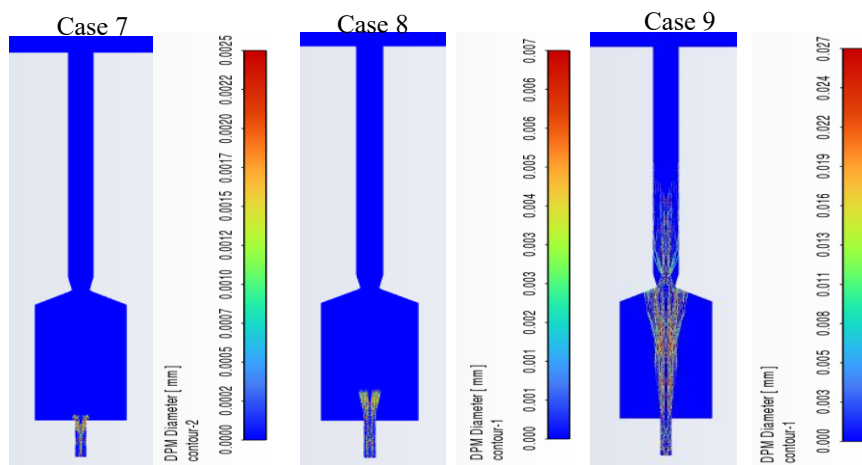


Figure 9. Droplet size distribution for uniform cases 7–9.

As illustrated in Figure (10), the uniform cases exhibit more localized evaporation and narrow high-temperature zones. This leads to sharper thermal gradients and a notable flame extension beyond the chamber. This contrasts sharply with the R-R cases, which maintain a broader and more confined flame structure, as previously demonstrated in the simulation results in Figure (9).

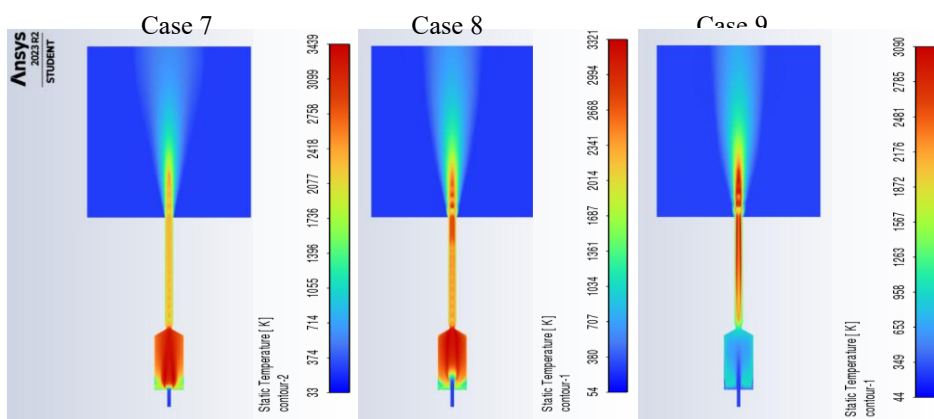


Figure 10. Temperature contours for uniform droplet cases 7-9.



4. Conclusions

This study successfully utilized Computational Fluid Dynamics (CFD) to investigate the profound impact of various droplet size distributions, modeled via the Rosin-Rammler (R-R) parameters ($\bar{d}$ and n), on the kerosene flame characteristics within a thermal spray environment. The model demonstrated strong agreement with experimental radial temperature profiles (Saadoun, 2023) specifically for the finer R-R distributions (Case 1 and Case 2), thereby validating the numerical approach for predicting reliable thermal fields. Analysis confirmed that the Mean Diameter ($\bar{d}$) is the dominant factor governing combustion: small $\bar{d}$ distributions (e.g., Cases 1 and 2) promoted rapid evaporation and concentrated heat release, resulting in a stable flame confined within the chamber. Conversely, large $\bar{d}$ distributions caused delayed evaporation and flame extension outside the chamber, significantly compromising efficiency. Furthermore, the polydisperse R-R distributions (which incorporate size variability) were found to be superior to the Uniform (monodisperse) cases. While uniform injection resulted in sharper thermal gradients and severe flame extension, the R-R cases, due to the continuous presence of droplets of varying sizes, maintained a broader, more confined, and stable flame structure, highlighting the practical advantage of realistic atomization for efficient thermal coating applications. These results provide a solid foundation for optimizing fuel injection strategies. For future work, it is recommended to integrate the validated R-R distributions into a fully coupled DPM model that includes the final solid particle melting and deposition process to directly link the combustion efficiency to the final coating characteristics. Furthermore, investigating the effect of R-R parameters on pollutant formation (e.g., NO_x and Soot) is essential for environmental compliance.

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