# Modeling and Simulation of Evaporating Water/Nitrogen Spray Using Direct Quadrature Method of Moments

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**Abstract**

Spray flows occur in many physical and chemical applications, for instance in combustion processes, spray drying processes, or environmental physics. The improved understanding of underlying processes that govern the dynamics of spray flows are critical to assure the reliability and performance of these systems. In particular, the process of evaporation is of key interest in these systems. The present work focuses primarily on study of droplet size distribution by means of direct quadrature method of moments (DQMOM), where DQMOM is extended to account for evaporating sprays by including an advanced convective droplet vaporization model. The results are compared with experimental data of an evaporating water spray carried by nitrogen.

## Introduction

The principal physical processes that are involved in spray systems are transport in physical space, droplet evaporation, acceleration of droplets due to drag and droplet collisions inducing breakup and coalescence. The evolution of particulate and other dispersed-phase systems can be modeled using population balance equation (PBE). The PBE is a continuity equation defined over a number density function. For spray systems, such PBE is proposed by Williams [1] based on kinetic theory. For its solution, quadrature method of moments (QMOM) has been studied as an attractive approach by defining the spray dynamics rather globally [2, 3, 4]. In QMOM, moment equations are approximated as weighted sum of radii by assigning higher weights to larger droplets that contribute more in transport and dynamics of system, using Guassian quadrature formulation based on product-difference algorithm developed by Gordon [2]. This approach has been validated [3] and extended [4] by Marchisio *et al.* to include the effects of aggregation and breakup.

However, while implementing it to realistic cases, two major problems have been faced. At first, it poses difficulties in treating the systems where dispersed phase velocity strongly depends upon internal coordinates of the system and secondly, numerical issues are quite challenging in case of bivariate (and multivariate) density functions which are characteristic in many technical applications. Thus to overcome these problems, DQMOM has turned out to be an attractive alternative [5], which is particularly efficient in cases of poly-dispersed multiphase flows. This approach is adapted in the present study for a water spray in nitrogen, and an advanced model to account for spray evaporation [7] is included. The initial values for starting the simulations have been taken from the experimental data provided by BASF, Ludwigshafen, where a water spray is injected through a hollow cone nozzle into a cylindrical spray chamber and carried by nitrogen. Droplet size distribution is measured at different cross sections of the spray chamber for constant inlet gas velocity at room temperature.

## Mathematical Model

The mathematical modeling is achieved through application of DQMOM to Williams spray equation [5]. The effects of evaporation have been included in the model by using the relation proposed by Abramzon and Sirignano [7]. A two-step MacCormack numerical sheme [6] is adapted to solve the system of equations obtained via DQMOM. At present, homogeneous solutions for DQMOM are obtained, where the initial data for simulations are taken from experiments. Calculations have been performed at 293 K and profiles of Sauter mean diameter and specific surface area are compared with experimental data at the same conditions. In order to analyze the effect of evaporation on the droplets, simulations have been carried out at different temperatures of surrounding gas. The present study focuses on the droplet evaporation for future modeling of spray drying processes, whereas coalescence, drag force and droplet collisions are currently neglected.

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## Results and Discussion

It is observed that Sauter mean diameter increases with time (see Figure 1) whereas specific surface area decreases, which is because of loss of smaller size droplets due to evaporation. Comparing with experimental data, it appears that DQMOM (marked DQ) predicts the changes in droplet size distribution quite precise than QMOM (marked Q), which reveals the higher level of accuracy of DQMOM.

It is further seen that droplet number density decreases with time due to evaporation (see Figure 2) but this reduction is not predicted by QMOM as realistic as DQMOM. This argument is supported by comparing its profiles with that of total mass density (not shown here), which reveals higher precedence of evaporation of larger size droplets in case of QMOM. Effects of evaporation on droplet number density are studied through its variation with time at different temperatures of surrounding gas. Though the difference in predictions of QMOM and DQMOM is decreasing with increase in temperature, but QMOM is vulnerable to reveal physically non significant solutions at large time such as negative weights [8].

Moreover, Sauter mean diameter and specific surface area are investigated at different temperatures of ambient gas (not shown here). All the studied parameters have constant profiles in case of no evaporation, which assures the accuracy of numerical schemes.

The model properly accounts for droplet evaporation, and droplet interactions will be implemented in future extension of the code.

## Acknowledgements

Financial support of the German Science Foundation (DFG) through SPP 1423 is gratefully acknowledged. RMH acknowledges financial support of Kohat University of Science and Technology, Pakistan. The authors thank Dr. Wengeler from BASF, Ludwigshafen, for providing the experimental data.

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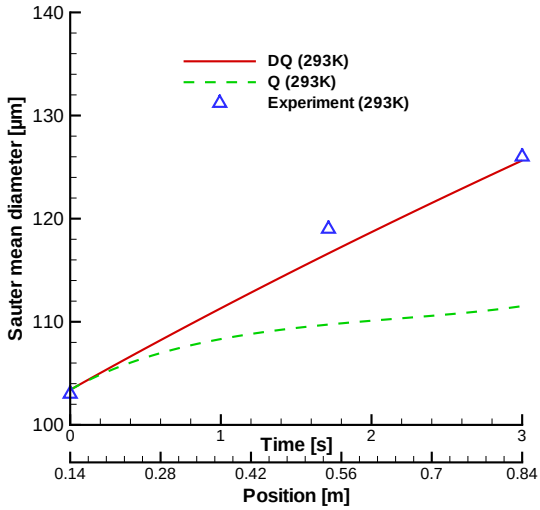


**Figure 1.** Time variation of Sauter mean diameter

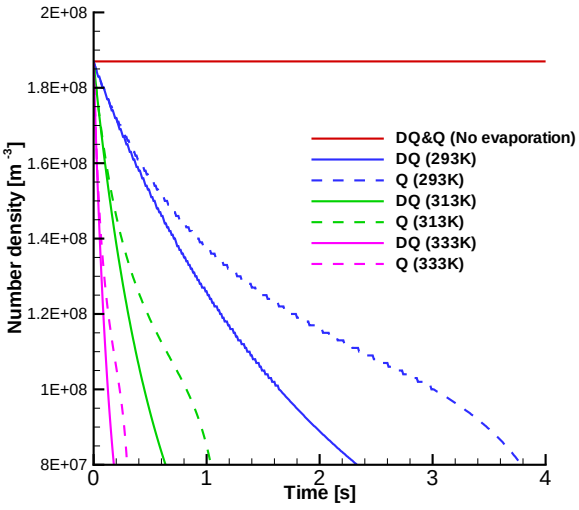


**Figure 2.** Effect of evaporation on number density