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## On the realizability and boundedness of the moments in a bubbly gas-liquid pipe flow

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## Abstract

The quadrature-based moment methods (QBMM) are widely used to solve the population balance equation (PBE), which provides a useful understanding of the evolution of disperse systems, e.g. bubbly gas-liquid flow. A key element of the methods is the moment-inversion algorithm that fails if the set of moments is not realizable. When the moment transport equations (derived from the PBE) include the convective term, employing standard high-order discretization schemes may cause the non-realizability problem. As a result, several realizable high-order schemes have been developed to address this issue. This work makes use of a bubbly developing pipe flow to investigate the performance of three schemes including 1<sup>st</sup>- and 2<sup>nd</sup>-order schemes, which can prevent the non-realizability problem. Eventually, the predictions will be discussed from the point of view of moment boundedness, a property that must be respected to obtain physical predictions.

## Introduction

The population balance equation (PBE) integrated with the Two-Fluid Model (TFM) provides a powerful tool to follow the evolution of the properties of the bubble population in a bubbly gas-liquid flow. PBE is a continuity statement of the Number Density Function (NDF) which describes how the bubble population is distributed in space and time. The quadrature-based moment methods (QBMM) are efficient approaches to solve the PBE where few low-order moments of the NDF are tracked by solving the moment transport equations. At the core of these methods is the approximation of the NDF by the summation of some weighted Dirac delta functions, each centered on a quadrature node. The weights and the nodes of the quadrature can be calculated from the moments via the so-called inversion algorithms. However, the approach fails when the set of moments is not realizable, i.e. there exists no NDF corresponding to such a set of moments. The main cause of the non-realizability problem is the scheme employed to discretize the convective term of the moment transport equation. Thus, developing schemes that preserve the realizability of the moments is of high importance. However, the schemes should also respect the boundedness of the moments as they are associated with some physical properties of the disperse phase. It is an important property of the moments that should not be overlooked. In this work, we will compare and discuss the predictions of the PBE applied to a bubbly pipe flow, using three schemes developed to overcome the non-realizability problem. They include the 1st-order upwind, the quasi-2nd-order realizable scheme (Vikas et al. 2001) and the equal-limiter scheme (Shiea et al. 2018). It will be shown that the equal-limiter scheme can improve the results in such a way to not only prevent the non-realizability issue but also respect the boundedness of the moments.

## **Test case and Simulation Approach**

The investigated test case (Bayer et al. 2008) is an air-water cocurrent flow inside an adiabatic (30 °C) vertical pipe with height of 8 (m) and inner diameter of 0.1953 (m), see Fig. 1. The water flows from the bottom and the air (at 2.5 bar) enters through the injection points embedded on the wall. A wire-mesh sensor located near the pipe outlet measures local air volume fraction, air velocity and bubble size distribution. The flow regime of the selected operating conditions is the bubbly flow regime.

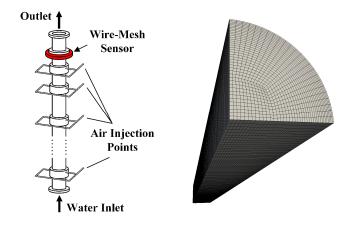


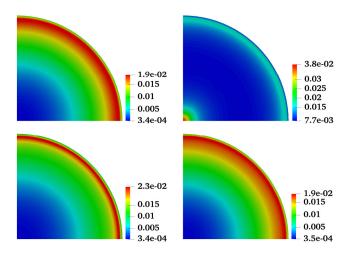
Figure 1: Left) Experimental setup; Right) Designed mesh.

The simulations are performed using the TFM solver of OpenFOAM v5.0, *twoPhaseEulerFoam*, coupled with the PBE as described by Buffo et al. (2016). Only the first 2 meters of the column was simulated since it is long enough to study the behavior of the numerical schemes. Taking advantage of the axial symmetry of the system, a quarter of the column is discretized by a structured O-grid mesh for performing the simulation (Fig. 1). The gas inlet is modelled by a ring of faces around the wall. The TFM considers the following interfacial forces acting on the bubbles: drag, lift, turbulent dispersion and wall lubrication. The details of the employed correlations and simulation settings can be found in our previous work (Shiea et al. 2019). The turbulence is considered only in the liquid phase and is modelled by the k- $\epsilon$  RANS model. Finally, the coalescence and the breakage of the bubbles are modelled on the assumption that the turbulence mechanism dominates.

Three discretization schemes for the convective term of the moment transport equation are studied: 1) the upwind scheme, which approximates the flux of the moments through each interface using the values of the upwind cell, 2) quasi-2<sup>nd</sup>-order realizable scheme (Vikas et al. 2011), which interpolates the quadrature nodes by the *upwind* scheme and the quadrature weights by the 2<sup>nd</sup>-order TVD *minmod* scheme. Then, it calculates the flux of the moments by reconstructing the moments from the interpolated values of the quadrature nodes and weights, 3) the equal-limiter scheme (Shiea et al. 2018), which applies the 2<sup>nd</sup>-order TDV *minmod* scheme directly to the moments, but it limits all moment fluxes equally using the minimum limiter among those calculated for all the moments.

#### **Results and Discussion**

Figs. 2 and 3 depict, respectively, the contour plots and radial profiles of the air volume fraction obtained by the TFM along with those predicted by the PBE using the mentioned discretization schemes. The results belong to a section located at the distance of 1.5 (m) from the air injection point. It is worth remarking that the moment of order three with respect to bubble size evaluated by the PBE is proportional to the air volume fraction evaluated by the TFM. In other words, the air volume fraction can be retrieved by multiplying the moment of order three and the volumetric shape factor, which is  $\pi/6$  for spheres. Moreover, the discretization scheme used by the TFM is the standard 2<sup>nd</sup>-order TVD *minmod* scheme, which is bounded. However, it is not possible to use the same scheme for the convection of the moments due to the non-realizability problem.



**Figure 2:** Contour plots of the air volume fraction obtained by TFM (top left); PBE with upwind scheme (top right), quasi-2<sup>nd</sup>-order scheme (bottom left) and equal-limiter scheme (bottom right)

The upwind scheme (top right in Fig. 2 and yellow line in Fig. 1) results in unsatisfactory predictions compared to the experiments due to the high numerical diffusion that occurs in the radial direction in this specific system, leading to an unphysical gas accumulation at the center of the column. Therefore, it is necessary to employ high-order schemes to decrease the numerical diffusion. The quasi-2<sup>nd</sup>-order scheme improves the accuracy of the predictions (bottom left in Fig. 2 and red line in Fig. 3), however, the comparison of its predictions with the bounded results of the TFM (blue line in Fig. 3) shows that it violates the boundedness of the air volume fraction. Finally, the predictions obtained by the equal-limiter scheme (bottom right in Fig. 2 and green line in Fig. 3) are very close to those obtained by the TFM. Moreover, its predictions are bounded as it applies the TVD scheme (with minimum limiter) directly to the moments.

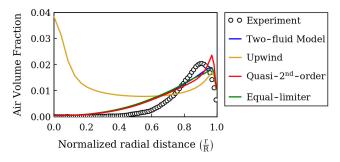


Figure 3: Radial profiles of the air volume fraction

#### Conclusions

Three discretization schemes, which can overcome the non-realizability problem, were tested in a bubbly pipe flow simulation. The necessity of employing high-order schemes was recognized since the 1<sup>st</sup>-order solutions were too diffusive to be acceptable, resulting in an unphysical behavior. Moreover, it was illustrated that applying high-order schemes to variables other than the moments, e.g. quadrature weights, may produce unbounded results, even if the scheme is itself bounded.

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