RESEARCH REPORT

VTT-R-00699-24

Further calibration of OpenFOAM polydisperse flow models

Authors: Petteri Peltonen, Juho Peltola, Timo Niemi, Ville Hovi

Confidentiality: VTT Public

Version: 1

beyond the obvious

Report's title	
Further calibration of OpenFOAM polydisperse flow models	
Customer, contact person, address Valtion ydinjätehuoltorahasto Linda Kumpula (Työ- ja elinkeinoministeriö) PL 32, 00023 Valtioneuvosto	**Order reference** Dnro SAFER 15/2024
Project name SAFER2028 CFD for Reactor Safety	**Project number/Short name** 138683/SAFER2028_CeReSa_2024
Author(s) Petteri Peltonen, Juho Peltola, Timo Niemi, Ville Hovi	**Pages** 12/–
Keywords Population balance model, turbulent dispersion, OpenFOAM	**Report identification code** VTT-R-00699-24

Summary

This report summarizes advancements in polydisperse flow modeling as part of the SAFER2028_CERESA_2024 project, building on the findings of the 2023 CeReSa project. In the previous work, we identified a critical limitation in the OpenFOAM polydisperse flow models: their inability to account for turbulent dispersion effects in bubble size distributions. To address this, it is proposed to calculate the turbulent dispersion separately for each size group in the population balance equations (PBEs).

The present report extends this work by refining the proposed model through calibration and evaluating its performance using more realistic and challenging test cases, such as the DEBORA benchmark. The results demonstrate significant improvements in capturing the void fraction and bubble size distributions, particularly in the ability to reproduce a centerline peak void fraction distribution in high-pressure, boiling flow conditions of the DEBORA experiment relevant to nuclear safety applications. While the implemented turbulent-dispersion-by-size-group enable prediction of centerline peak void fraction profile, the present implementation is still incomplete in terms of consistency between the phase fraction and size group transport. This should still be addressed, before more comprehensive model calibration or validation is attempted.

This work advances the predictive accuracy of CFD simulations for multiphase flows and underscores the importance of experimental validation in developing reliable models for nuclear safety assessments.

Confidentiality	VTT Public

Espoo

Written by	Reviewed by
Petteri Peltonen, Research Scientist	Timo Pättikangas, Research Team Leader

VTT's contact address

VTT Technical Research Centre of Finland Ltd, P.O. Box 1000, FI-02044 VTT, FINLAND

Distribution (customer and VTT)

SAFER2028 Technical Advisory Group 2.1, Petteri Peltonen (VTT), Timo Niemi (VTT), Juho Peltola (VTT), Ville Hovi (VTT), VTT archive

Approval

VTT TECHNICAL RESEARCH CENTRE OF FINLAND LTD

Date:	03/02/2025
Signature:	
Name:	Francesco Reda
Title:	Research Manager, Energy

Contents

1. Introduction

Computational Fluid Dynamics (CFD) has been successfully utilized in nuclear safety assessments, offering a comprehensive evaluation of factors such as thermal-hydraulic performance, containment stability, and the behavior of radioactive materials under different operational conditions. Experimental methods often face limitations when it comes to capturing the intricate fluid dynamics within the complex geometries of nuclear reactors and related systems. CFD simulations address these challenges by providing detailed insights into the thermal-hydraulic behavior of reactor cores, coolant pathways, and containment structures. This information is essential for assessing safety margins and identifying potential vulnerabilities under both normal and accident scenarios.

In particular, containment studies often involve phenomena that require modeling the transport of particles of various sizes, such as sprays, aerosol movement, and boiling. In the context of severe accidents, CFD simulations are indispensable for predicting the behavior of released radioactive substances. They assist in emergency response planning and in reducing potential consequences by analyzing dispersion patterns and transport mechanisms of airborne contaminants. Such insights are crucial for developing effective strategies to protect both plant workers and the public.

Modeling complex, interconnected phenomena—such as inter-phase forces in multiphase systems, their influence on flow, and the resultant heat and mass transfer—necessitates the inclusion of multiple closure models within CFD simulations. Selecting appropriate closure models is often challenging because the interactions among them can lead to unpredictable behavior. Additionally, these models often include parameters that require calibration against experimental data. Identifying which model is responsible for a specific effect, or predicting how a particular parameter adjustment or model choice will alter results, is a complex task. This complexity becomes even more pronounced when validating CFD models against experimental results from integral test facilities, where multiple phenomena occur simultaneously.

These challenges underline the importance of ongoing efforts in model development and validation. Reducing uncertainties in computational modeling is essential to improving the reliability of CFD simulations, thereby enhancing their role in nuclear safety assessments.

2. Modelling of polydisperse multiphase flows

2.1 Population balance modelling

Following [1, 2], in OpenFOAM, the population balance equation (PBE) governs the distribution of dispersed particles, tracking their dynamics across different size groups. The general transport equation for the particle number density, N_i, is given by:

$$\frac{\partial N_i}{\partial t} + \nabla \cdot (\mathbf{U}_d N_i) = H_i, \tag{2.1}$$

where $\mathbf{U}_d$ is the velocity of the dispersed phase, and H_i represents source terms such as coalescence, breakup, or mass transfer.

To facilitate analysis, particle concentrations are expressed in terms of volume concentrations:

$$\alpha_i = v_i N_i, \tag{2.2}$$

where v_i is the representative particle volume. Summing over all size groups yields the total volume fraction of the dispersed phase:

$$\alpha_d = \sum \alpha_i. \tag{2.3}$$

While the total dispersed phase volume fraction, α_d, is solved as part of the multiphase flow module (e.g., `multiphaseEuler`), the PBE determines how the dispersed phase is distributed across size groups. This is achieved using size group fractions:

$$f_i = \frac{\alpha_i}{\alpha_d}, \tag{2.4}$$

which are constrained by the following conditions:

$$0 \leq f_i \leq 1, \quad \sum_i f_i = 1. \tag{2.5}$$

Expressing the PBE in terms of size group fractions gives:

$$\frac{\partial(\alpha_d f_i)}{\partial t} + \nabla \cdot (\alpha_d \mathbf{U}_d f_i) = S_{ij}, \tag{2.6}$$

where S_{ij} represents intergroup source terms describing coalescence, binary breakup, or other mechanisms responsible for transferring particles between size groups.

To address cases where particle velocity depends on size, the dispersed phase can be divided into multiple velocity groups, each with a distinct velocity field, $\mathbf{U}_\varphi$. The total dispersed phase fraction is then:

$$\alpha_d = \sum_{\varphi \in d} \alpha_\varphi, \tag{2.7}$$

and the size group fractions within each velocity group are redefined as:

$$f_{i,\varphi} = f_i \frac{\alpha_d}{\alpha_\varphi}. \tag{2.8}$$

For each size group i in velocity group φ, the PBE becomes:

$$\frac{\partial(\alpha_\varphi f_{i,\varphi})}{\partial t} + \nabla \cdot (\alpha_\varphi \mathbf{U}_\varphi f_{i,\varphi}) = S_{ij,\varphi}. \tag{2.9}$$

The source terms $S_{ij,\varphi}$ account for both particle transfer between size groups within a velocity group and interactions at the interface between velocity groups.

2.2 Additional turbulence treatment

In the previous report [3] we illustrated the inability of the PBE model in OpenFOAM Foundation release to take into account the modelled turbulence effects in the size group transport equations. This inability is again shown in Figure 1, where a set of different size bubbles is injected into turbulent channel flow. Without any additional treatment, the bubbles do not mix at all, which is clearly non-physical but expected result as the PBE doesn't include any turbulent dispersion terms, although the turbulent dispersion term is include in the phase momentum equations.

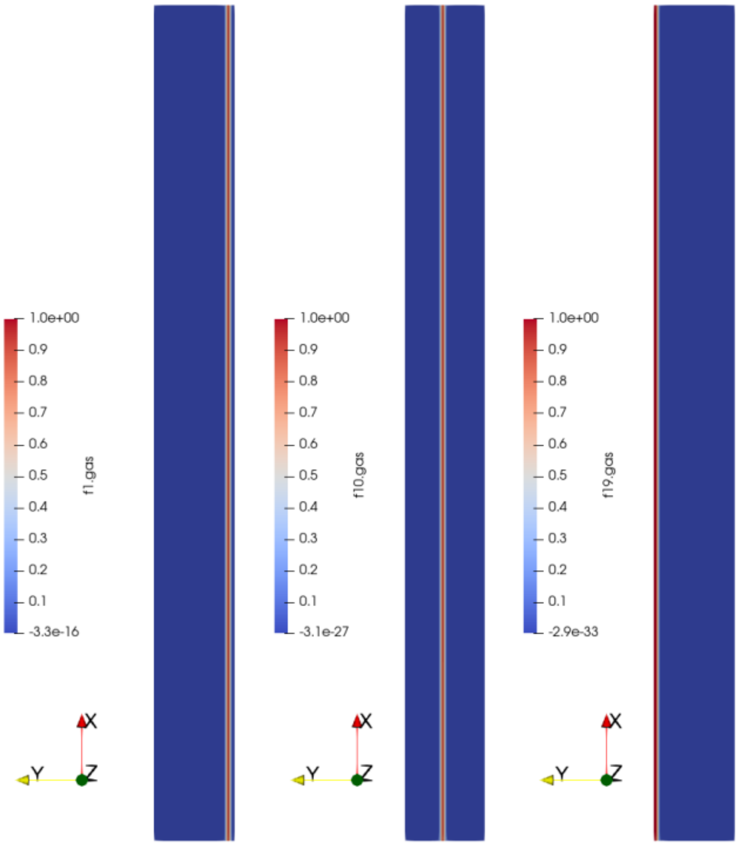

Figure 1. Bubble size distributions of different size bubbles injected into turbulent flow, without additional turbulence treatment in the size group transport equations.

During the 2023 project, we proposed an additional correction term to be added to the size group transport equations

$$\frac{\partial(\alpha_\varphi f_{i,\varphi})}{\partial t} + \nabla \cdot (\alpha_\varphi \mathbf{U}_\varphi f_{i,\varphi}) - \underbrace{\nabla^2 (D_i \alpha_\varphi f_{i,\varphi})}_{correction} = S_{ij,\varphi}. \tag{2.10}$$

In Eq. 2.10 $D_i = \nu_T / Sc_i$ is a size-group specific diffusion coefficient with a user-input turbulent Schmidt number Sc_i. The effect of the correction term is illustrated in Figure 2 where the injected bubbles mix due to turbulence.

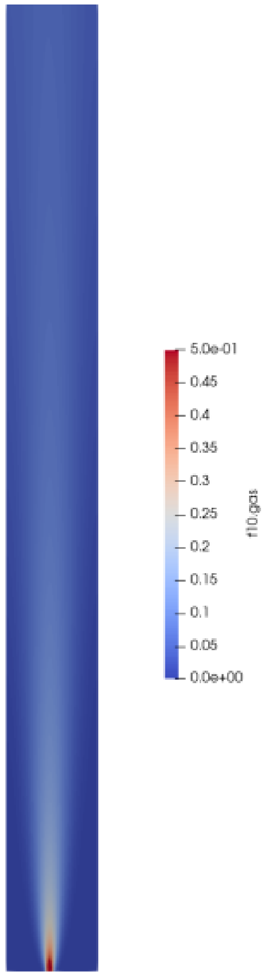

Figure 2. Bubble size distribution with the additional turbulence treatment presented in the previous project.

While the proposed correction term was shown to more physically mix the size groups due to modelled turbulence, we also showed [3] that while the flux $\alpha_{varphi} f_i$ is conserved, the addition may result in the size groups f_i to diffuse out of the phase they belong to. To mitigate the issue, we propose taking into account the turbulent dispersion of the size groups with an additional turbulent dispersion term in the *momentum* transport equation of the phase. The added turbulent dispersion force term for phase j is

$$F_{jn} = \sum_i K_{jn} D_i \nabla(\alpha_j f_i), \tag{2.11}$$

where K_{jn} is the drag between phases j and n. We note that the implementation is carried out using the `liftModel` model interface in OpenFOAM since it supports arbitrary forces to be added to the momentum equations.

3. Turbulent dispersion by size group approach

For the present simulations of the DEBORA boiling cases, a new approach was adopted. Following the example of implicit phase pressure treatment of turbulent dispersion in OpenFOAM, which enables implicit treatment of the phase fraction gradient of the turbulent dispersion force in the phase fraction equation.

In this approach, the phase fluxes, ϕ_φ, are first modified by removing a dispersion flux:

$$\phi_{*,\varphi} = \phi_\varphi + DbyA_{sum}[\nabla(\alpha_\varphi)]_{f,\perp} \tag{3.1}$$

where subscript f indication variable value on cell faces and subcript $\perp$ face normal gradient. $DbyA_{sum}$ is sum over all active turbulent dispersion models between phases φ and ψ that adds together contributions from each phase pair. $D_{TD,\varphi}$ is the dispersion coefficient for phase pair φ, ψ, and A_φ is the diagonal part of the matrix origination from the discretization of the phase momentum equation.

$$[DbyA_{sum}]_f = \sum_{\varphi,\psi \in D_{TD,\varphi,\psi}} \frac{\alpha_{\varphi,f}\alpha_{\psi,f}}{\alpha_{\varphi,f} + \alpha_{\psi,f}} \left[\frac{D_{TD,\varphi,\psi}}{max(A_\varphi, A_\psi)}\right]_f \tag{3.2}$$

The phase fraction transport is then solved explicitly using the MULES algorithm and the modified fluxes. The previously removed dispersion flux is then re-introduced to the phase fraction transport in α implicit manner by solving

$$\left[\frac{\partial(\alpha_\varphi f)}{\partial t}\right]_i - \left[\frac{\partial(\alpha_\varphi f)}{\partial t}\right]_e - \nabla \cdot [DbyA_{sum}]_f \nabla\alpha_\varphi \tag{3.3}$$

Important to note here is that all the phases use the same $[DbyA_{sum}]_f$ which is needed to ensure consistency of the phase fluxes and thus conservation.

In the following an approach resembling this is adopted to define the diffusion coefficients in the PBEs. The main motivation to investigate the influence of the population balance turbulence dispersion on the DEBORA experiment is to the see if the transition form the near wall void fraction peak to center line volume fraction peak observed in the experiments can be reproduced by introducing the turbulent dispersion calculation on individual size group level. To observe the effect in full not only the gradient in Eq. 2.10 dispersion term, but also the dispersion coefficient is evaluated by size group. Thus, the approach used in the phase fraction equations and described above cannot be directly applied and the approach used here leads to inconsistencies in size group and phase fraction transport. However, it should serve the purpose of demonstrating that in the DEBORA experiment and similar wall boiling applications, the transition from near wall void fraction peak to center line peak can be achieved by inclusion of turbulent dispersion modeling on population balance size group level, and without any accompanying changes to modeling of other non-drag forces: lift, wall lubrication force or virtual mass force.

For the present results, the PBEs were modelled as

$$\frac{\partial(\alpha_\varphi f_{i,\varphi})}{\partial t} + \nabla \cdot (\alpha_\varphi \mathbf{U}_\varphi f_{i,\varphi}) - \underbrace{\nabla^2(D_i f_{i,\varphi})}_{correction} = S_{ij,\varphi}. \tag{3.4}$$

Where

$$D_i = \frac{\alpha_\varphi f_{\varphi,i,f}\alpha_{cont,f}}{\alpha_{\varphi,f} f_{\varphi,i,f} + \alpha_{cont,f}} \left[\frac{K_{i,\varphi,cont}\nu_{t,cont}/\sigma_{TD}}{max(A_\varphi, A_{cont})}\right]_f \tag{3.5}$$

Here, $K_{i,\varphi,cont}$ is the phase intensive momentum transfer coefficient between the bubbles if this size group - evaluated using the representative diameter of the group - and the continuous liquid phase. $\nu_{t,cont}$ is the turbulent viscosity of the continuous liquid phase and σ_{TD} a model parameter that is the same for all the size groups and varies 0.1...1. In the present simulation σ_{TD} = 0.1 was used.

4. Debora benchmark results

In this section, we present simulation results from the Debora benchmark using the newly implemented models. Details of the Debora benchmark can be found in the previous report [3]. The benchmark consists of a heated pipe operating under high-pressure conditions relevant to nuclear safety. As liquid flows through the pipe, heat applied at the walls causes boiling, resulting in the formation of bubbles of varying sizes.

Figure 3 illustrates the results for Debora benchmark 1 (p = 2.62 MPa, q = 73890 W/m^2, σ = 0.00176 N/m) without the turbulence treatment corrections introduced in this report. The comparison between simulation and experimental results shows reasonable agreement. While minor deviations are observed in both the void fraction and mean bubble diameter near the wall, the overall correspondence is satisfactory. This case and these results are the "wallBoilingPolydisperseTwoGroups" turorial provided with OpenFOAM Foundation release 12.

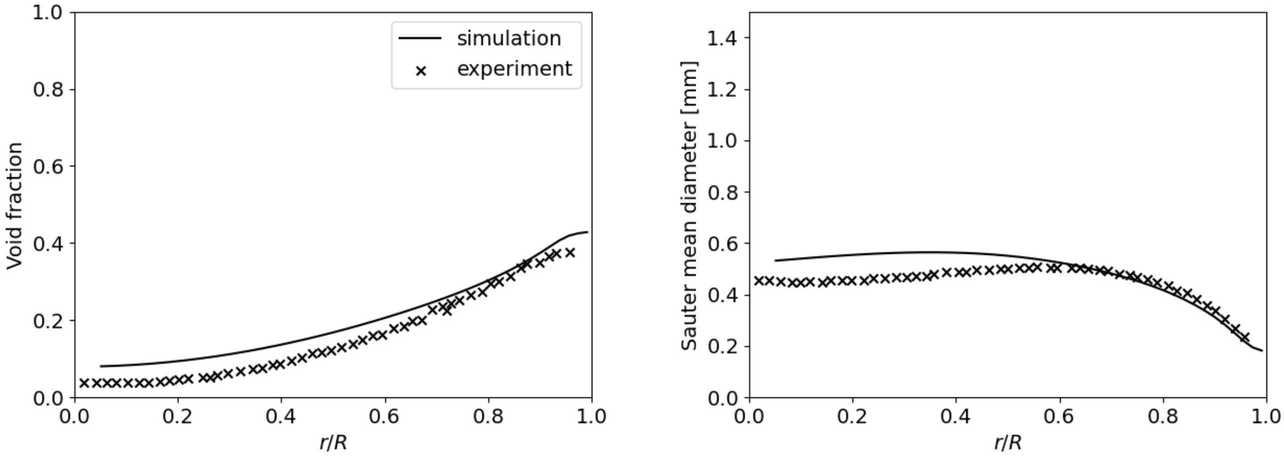

Figure 3. Simulation results compared to experiments for Debora benchmark 1 without turbulence treatment corrections for size group fractions.

Using the same modeling setup for simulations of Debora benchmark 6 (p = 1.459 MPa, q = 76260 W/m^2, σ = 0.00467 N/m) with couple of parameter varations (turbulent dispersion C_{TD} = 0.1 instead of 1.0 and using the default $C1$ = 0.356 for the Prince-Blanch coalescence model, instead of the adjusted value used in the tutorial case) reveal significant deviations from experimental data, as shown in Figure 4. Notably, the void fraction at the wall is drastically overpredicted, and the simulation results exhibit a completely different trend compared to the experimental data. This pronounced mismatch in void fraction motivates the introduction of correction terms, as presented in this report.

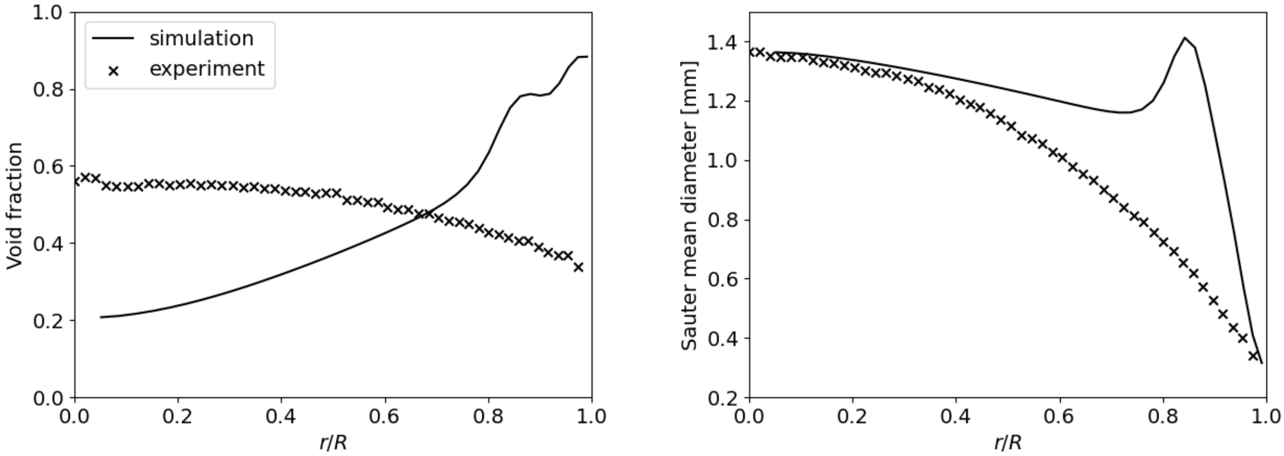

Figure 4. Simulation results compared to experiments for Debora benchmark 6 without turbulence treatment corrections for size group fractions.

By incorporating the correction terms proposed in equations 3.4 and 2.11, the void fraction in Debora benchmark 6 aligns much more closely with the experimental results (see Figure 5). Most significantly, the near wall void fraction peak of the previous results has been replaced with center-line void fraction peak which is similar to the experimental result. This shows, that the transition between these two modes can be effected by inclusion of the turbulent dispersion of size group level, without modification of the other interfacial force models: lift, wall lubrication, drag or virtual mass forces.

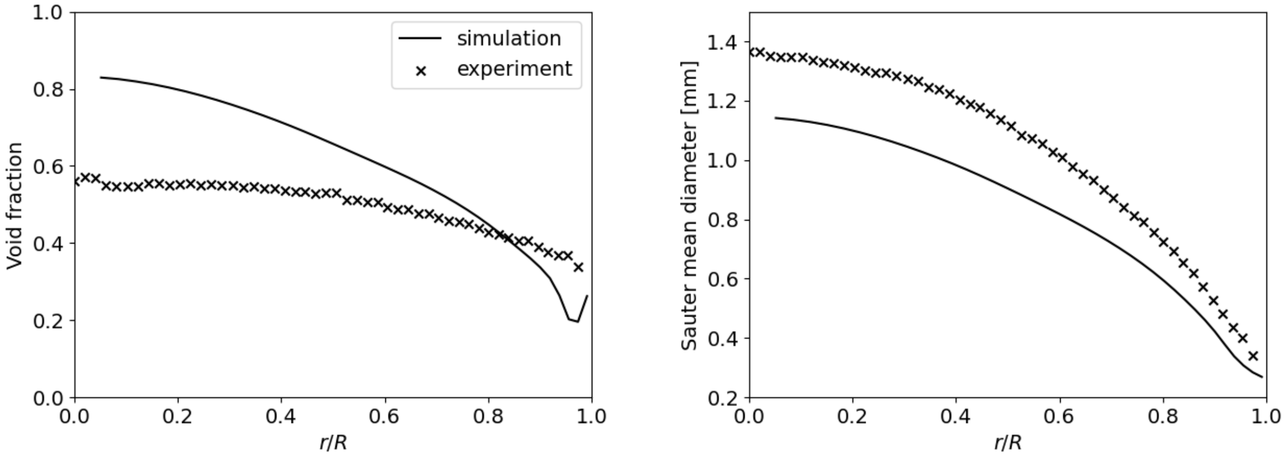

Figure 5. Simulation results compared to experiments for Debora benchmark 6 with turbulence treatment corrections for size group fractions.

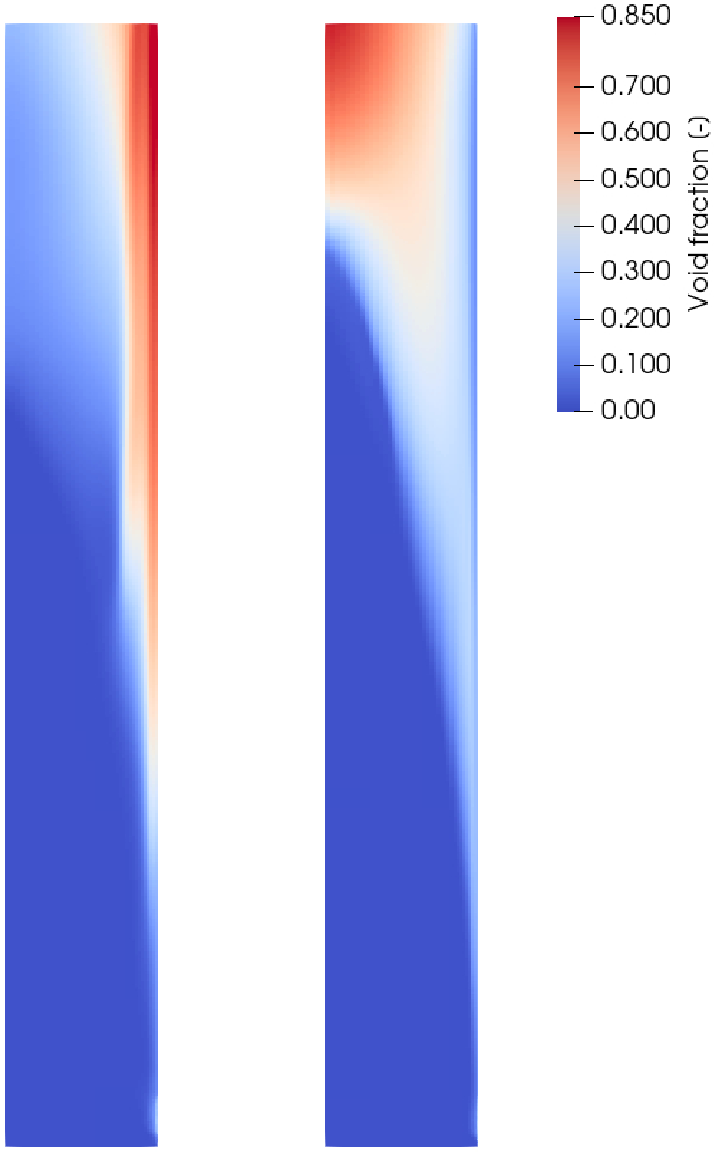

Figure 6. The Debora benchmark case 6 bubble void fraction fields without dispersion in PBEs (left) and with the turbulent dispersion included in the PBEs by size group (right). The flow direction is upwards and the heated wall boundary is on the right. The domain has been vertically shrunk by 1:50 for visualization purposes.

5. Conclusion

This report presented advancements in modeling polydisperse multiphase flows using population balance equations (PBEs) within the OpenFOAM framework, with a particular focus on addressing challenges in nuclear safety applications. Specifically, we examined the Debora benchmark as a case study to evaluate the performance of the proposed models under high-pressure boiling conditions.

The results demonstrated that the baseline implementation of PBEs without turbulence treatment failed to adequately capture the experimental trends in certain scenarios, such as the DEBORA experiments. In simulations of the DEBORA experiments the model combination (similar to models used in the DEBORA tutorial case included with the OpenFOAM Foundation releases and widely in the literature) tend to predict a near wall void fraction maximum in all operational points. Thus failing to reproduce the shift to center-line void fraction maximum that is observed in experimental points where the overall void fraction is high.

Previously [3] it was highlighted that the population balance model does not include turbulent dispersion effects in the size group transport equations and that this can lead to clearly unphysical behavior. Different approaches to improve the behavior were also discussed in the report. In the present work, the effect of including the turbulent dispersion in the PBEs is investigated in context of wall boiling simulations with hypothesis that neglecting the effect is a significant factor why the models tend to fail the predict the transition between the near wall and center-line void maximums.

To mitigate these issues, two major corrections were introduced: (1) the addition of a diffusion term to the size group transport equations, incorporating turbulence effects via a size-specific diffusion coefficient, and (2) a turbulent dispersion force in the momentum equations, ensuring that size group fractions remain consistent within the dispersed phase. These changes significantly improved the result in a high void fraction operational point (Case 6). Most significantly, the near wall void fraction peak of the previous results was replaced with center-line void fraction peak which is similar to the experimental result.

The present implementation of the size group level turbulent dispersion calculation leads to inconsistencies in size group and phase fraction transport. Thus, as presented it cannot be recommended for general use and these inconsistencies should be addressed before more extensive verification, calibration and validation efforts are carried out. However, it should serve the purpose of demonstrating that in the DEBORA experiment and similar wall boiling applications, the transition from near wall void fraction peak to center line peak can be achieved by inclusion of turbulent dispersion modeling on population balance size group level, and without any accompanying changes to modeling of other non-drag forces: lift, wall lubrication force or virtual mass force.

The study also emphasized the importance of experimental validation in identifying deficiencies in computational models and guiding their improvement. While the proposed corrections demonstrate the importance and potential of addressing key shortcomings, they also introduced new challenges in numerics and physical modeling. The next step should be to improve the numerical implementation to ensure consistency of transport between the phase fraction and population balance transport equations, followed by testing in wider range of flow conditions.

References

[1] Robin Lehnigk et al. Population balance modelling with openfoam: Implementation and application to multiphase flows. *Chemical Engineering Science*, 227:115886, 2020.

[2] Ronald Lehnigk, William Bainbridge, Yixiang Liao, Dirk Lucas, Timo Niemi, Juho Peltola, and Fabian Schlegel. An open-source population balance modeling framework for the simulation of polydisperse multiphase flows. *AIChE Journal*, 68(3):e17539, 2022.

[3] Petteri Peltonen, Timo Niemi, and Ville Hovi. On modelling of turbulent dispersion in polydisperse flows. Technical Report VTT-R-00808-23, VTT Technical Research Centre of Finland Ltd, Espoo, Finland, January 2024. Prepared for Valtion Ydinjätehuoltorahasto. Reviewed by Juho Peltola. Distributed to SAFER2028 Technical Advisory Group 2.1. Confidentiality: VTT Public.