A Delayed Detached Eddy Simulation Model with Low Reynolds Number Correction for Transitional Swirling Flow in a Multi-Inlet Vortex Nanoprecipitation Reactor

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Abstract

The objective of the presented work is to verify a delayed detached eddy simulation (DDES) model for simulating transitional swirling flow in a micro-scale multi-inlet vortex reactor (MIVR). The DDES model is a k-ω based turbulence model with a low Reynolds number correction applied to the standard k-ω model such that the Reynolds-averaged Navier-Stokes (RANS) component of the DDES model is able to account for low Reynolds number flow. By limiting the dissipation rate in the k-equation, the large-eddy simulation (LES) part of the DDES model behaves similarly to a one-equation sub-grid model. The turbulent Reynolds number is redefined to represent both modeled

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Introduction

Manufacturing nanoparticles as a drug delivery platform requires a reproducible, scalable, and stable fabrication process. Anti-solvent precipitation such as Flash NanoPrecipitation (FNP) has been proven to be one of the most robust and scalable processes.\textsuperscript{1} The multi-inlet vortex reactor (MIVR) is a confined geometry chemical reactor specifically developed for controlling functional nanoparticle formation in the FNP process\textsuperscript{2,3} The MIVR used for producing functional nanoparticles is usually constructed with a reactor zone on the order of one millimeter in diameter. At the dimensions investigated here, this reactor is typically referred to as the micro-scale MIVR to avoid any potential confusion with scaled up MIVR reactors of similar geometry.\textsuperscript{4–6} Compared to other precipitation reactor geometries, such as the confined impinging jet reactor (CIJR), the micro-scale MIVR has the flexibility of controlling mixing ratios of solvents through various combination of inlet flow rates as all of the inlet streams contribute independently to the mixing in the chamber.\textsuperscript{2} Note that in processes where backmixing is desirable, the CIJR may be advantageous to the MIVR due to the more prevalent backmixing in the CIJR. Many applications have been reported as successfully producing functional nanoparticles by using the micro-scale MIVR, proving the broad applicability of the MIVR in anti-solvent precipitation processes.\textsuperscript{3,7–11}

The design and optimization of the micro-scale MIVR for nanoparticle production could
be greatly enhanced by developing reliable computational models of the flow and mixing in the reactor. Indeed, some work has been performed using computational fluid dynamics (CFD) to understand the flow characteristic and nanoparticle formation inside the micro-scale MIVR.\textsuperscript{2,9,12–14} Unlike many micro-scale chemical reactors which operate in the laminar flow regime, mixing in the micro-scale MIVR is enhanced by introducing turbulence into the flow. However, the introduction of turbulence makes development of computational models for the micro-scale MIVR challenging. Before developing any advanced computational models with regards to mixing and particle precipitation, the simulations of the flow inside the micro-scale MIVR must accurately predict flow quantities such as the mean velocity and turbulent statistics. In previous studies, Cheng et al.\textsuperscript{12} and Bensaid et al.\textsuperscript{9} applied both Reynolds Average Navier-Stokes (RANS) and Large Eddy Simulation (LES) approaches to simulate the turbulent flow inside the micro-scale MIVR with comparison to the microscope particle image velocimetry (micro-PIV) data. Shi et al. further studied the turbulent flow field inside the micro-scale MIVR in detail by using the micro-PIV technique.\textsuperscript{15} While previous simulations may provide some understanding about the flow field inside the micro-scale MIVR, RANS based turbulence models such as the $k$-$\epsilon$ or $k$-$\omega$ model do not provide accurate predictions for flow quantities such as the mean tangential velocity or turbulence statistics. This difficulty persists in both the micro-scale and scaled up MIVR. Indeed, Liu et al. pointed out that RANS and LES approaches may both fail to predict the turbulent swirling flow in a scaled-up MIVR.\textsuperscript{6} The RANS approach is inherently unable to predict transitional and/or swirling flow well because the RANS model is typically developed for highly turbulent flow and curvature effects in the MIVR are not adequately accounted for even using curvature correction models. The reason LES fails is primarily because the mesh resolutions must be incredibly fine for it to provide accurate predictions of flow in the MIVR, and these fine grids require a great many cells that make simulations prohibitively expensive.

Considering flow inside the micro-scale MIVR, for most of its applications it falls into the transitional flow region, i.e., both laminar and turbulence flow exists inside the reactor.
Specifically, laminar flow is introduced into the reactor (Reynolds number (Re) is usually far below 1000 in the inlets), and flow becomes turbulent as it spirals through the reactor and accelerates as it moves towards the outlet. Transitional flow is difficult to predict by using either the RANS or the LES approach. The ability of LES to predict transitional separated flow has been investigated with particular emphasis on the response to free-stream turbulence.\(^\text{16}\) It has been found that LES can yield a credible representation of transition induced by a combination of free-stream turbulence and separation. However, inadequate mesh resolution and the use of SGS modelling reduce the accuracy of LES predictions. For most flows of engineering interest, LES is still prohibitively expensive. To provide an affordable prediction tool, RANS models for transitional flow have been developed, and these models primarily fall into two categories, low Reynolds number (low-Re) turbulence models and intermittency-based models. By adding a low Reynolds number correction to a regular turbulence model, the transitional behaviour of flow can be predicted at the correct location.\(^\text{17}\) However, Menter et al. pointed out that a low-Re turbulence model is not capable of capturing the influence of factors that affect transitional behaviour such as separation.\(^\text{18,19}\) Intermittency-based models have been developed to avoid the disadvantages of low-Re turbulence models by incorporating local variables and empirical correlations.\(^\text{19}\) Recently, Ge et al. developed an intermittency model without using external data correlations.\(^\text{20}\) Nevertheless, in RANS models for transitional flow, a priori knowledge of the transition location or empirical correlations must be known, limiting their ability for accurately modeling flow away from its original test case.\(^\text{21}\)

It is especially challenging for the RANS approach to accurately predict the transitional swirling flow in the micro-scale MIVR. The main drawback to LES is the high computational cost caused by the fine mesh, especially near the wall. The Detached Eddy Simulation (DES) approach is a promising alternative method which improves the prediction capabilities of the RANS approach while requiring less computational resources compared to LES.\(^\text{22}\) The original DES model based on the Spalart-Allmaras model could have practical issues
such as artificial grid-induced separation and logarithmic-layer mismatch. Delayed DES was proposed to solve the artificial grid-induced separation by using a shielding function to prevent the RANS mode switching to LES mode near boundary layers.\textsuperscript{23} DDES can also incorporate other two-equation RANS models to improve the performance of its RANS component.\textsuperscript{24} In the DDES approach, a logarithmic-layer mismatch can be alleviated by modifying the length scale in the eddy resolving regions.\textsuperscript{25} Recently, DDES with a dynamic procedure has been developed and applied to simulate the turbulent swirling flow in a scaled-up MIVR with good agreement between simulation and experimental results.\textsuperscript{6,26}

Investigations on using DDES for transitional flows are lacking. Accordingly, a new DDES model is proposed in the current study to simulate the transitional flow within the micro-scale MIVR. In the new DDES model, a low Reynolds number k-ω model is used as the RANS mode. When the computational mesh is fine enough away from the wall region, the RANS mode will switch to the LES mode with a one equation sub-grid model. In the presented paper, the new DDES model is first derived. Then, the new DDES model is used to model the transitional flow in the micro-MIVR at different Reynolds numbers where experimental data will be used to validate the performance of the transitional DDES model.

Model formulation

The objective of the new DDES model is to use a low Reynolds number k-ω model in the laminar and transitional flow region and an LES model in the turbulent flow region. The low-Re k-ω model used here was derived by Wilcox\textsuperscript{17} and has proven to work well for low Reynolds number flow. The ability of the DDES model in predicting the transitional behavior of a flow is dependent on the capabilities of the low-Re k-ω model. Separation and streamline curvature effects in the flow are handled by the LES part of the DDES model. The derivation of the DDES model follows.

For incompressible flow, the dimensionless filtered Navier-Stokes equations can be ex-
pressed as (repeated indices imply summation)

\[ \frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (1) \]

\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial \bar{u}_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} \quad (2) \]

where \( \tau_{ij} \) is the Reynolds-stress tensor in the RANS approach and turbulent sub-grid stress tensor in the LES approach. It is modelled as

\[ \tau_{ij} = 2(\nu + \nu_T)S_{ij} - \frac{2}{3}k\delta_{ij} \quad (3) \]

where \( \nu \) is the kinematic viscosity, \( \nu_T \) is the turbulent kinematic viscosity that must be modelled, and \( S_{ij} \) is the filtered strain-rate tensor. \( k \) is the turbulent kinetic energy in the RANS approach and the sub-grid scale kinetic energy in the LES approach. The original k-\( \omega \) RANS model\(^\text{17} \) for modelling the turbulent viscosity can be written as

\[ \frac{Dk}{Dt} = 2\nu_T |S|^2 - C_\mu k\omega + \nabla \left[ (\nu + \sigma_k \nu_T) \nabla k \right] \quad (4) \]

\[ \frac{D\omega}{Dt} = 2C_\omega_1 |S|^2 - C_\omega_2 \omega^2 + \nabla \left[ (\nu + \sigma_\omega \nu_T) \nabla \omega \right] \quad (5) \]

where \( \nu_T = k/\omega \). The constants in the k-\( \omega \) model are

\[ C_\mu = 0.09, \sigma_k = 0.5, \sigma_\omega = 0.5, C_\omega_1 = 5/9, C_\omega = 3/40. \quad (6) \]

To improve its ability for predicting transitional flow, a low Reynolds number correction can be applied to the original k-\( \omega \) model.\(^\text{17} \) The low Reynolds number correction is applied by modifying the turbulent kinematic viscosity and the parameters \( C_\mu \) and \( C_\omega_1 \) such that

\[ \nu_T = \alpha^* \frac{k}{\omega}, \alpha^* = \frac{\alpha_0 + Re_T/R_k}{1 + Re_T/R_k}, C_\mu = 0.09 \frac{5/18 + (Re_T/R_\beta)^4}{1 + (Re_T/R_\beta)^4}, C_\omega_1 = \frac{5 \alpha_0 + Re_T/R_\omega}{1 + Re_T/R_\omega} \frac{1}{\alpha^*} \quad (7) \]
The constants for the low Reynolds number correction are

\[ R_\beta = 8, \alpha_0 = 1/10, R_\omega = 2.7, \alpha_0^* = 1/40, R_k = 6. \] (8)

The turbulent Reynolds number, \( R_{\text{eT}} \), is introduced here to represent the intensity of local turbulence. The relationship between \( R_{\text{eT}} \) and \( \alpha^*, C_\mu, C_\omega \) can be seen in Fig. 1. It can be seen that the low-Re correction is dependent on \( R_{\text{eT}} \), and all three modified coefficients will return to their original values at high Reynolds number when \( R_{\text{eT}} \) is approximately larger than 100. The definition of \( R_{\text{eT}} \) will be further discussed later.

Although it can be used to predict flow in channel and boundary layer applications, the \( k-\omega \) model with low Reynolds number correction has been criticized for being incapable of capturing factors such as separation and streamline curvature that affect transition.\(^{18,19}\)

Instead of using a correlation-based RANS model, it is proposed here to use a DDES model based on the low Reynolds number \( k-\omega \) model to account for factors that affect transition. The basic idea is to apply LES in the high turbulence region so that factors such as separation and streamline curvature can be captured and apply the low Reynolds number \( k-\omega \) model in the laminar region to predict the onset of transition. The proposed DDES model is based on the low Reynolds number \( k-\omega \) model where the dissipation in the \( k \)-equation is clipped by using length scale \( \ell_{\text{DDES}} \).

\[
\frac{Dk}{Dt} = 2\nu_T |S|^2 - \frac{\sqrt{k^3}}{\ell_{\text{DDES}}} + \nabla[(\nu + \sigma_k \nu_T)\nabla k] \] (9)

The DDES length scale \( \ell_{\text{DDES}} \) is defined as

\[
\ell_{\text{DDES}} = \ell_{\text{RANS}} + f_d \max(0, \ell_{\text{RANS}} - \ell_{\text{LES}}), \ell_{\text{RANS}} = \frac{\sqrt{k}}{C_\mu \omega}, \ell_{\text{LES}} = C_{\text{DES}} \Delta \] (10)

The DDES shielding function \( f_d \) is defined as
\[ f_d = 1 - \tanh([8r_d]^3), r_d = \frac{\nu_T + \nu}{\kappa^2 d_w \sqrt{U_{i,j} U_{i,j}}} \]  \hspace{1cm} (11)

where \( \kappa \) is the von Kármán constant, \( d_w \) the wall distance, and \( U_{i,j} \) the velocity gradient tensor. \( \Delta \) is an appropriate measure of grid size and is defined as

\[ \Delta = f_d V^{1/3} + (1 - f_d) h_{\text{max}} \]  \hspace{1cm} (12)

where \( V \) is the cell volume and \( h_{\text{max}} = \max(\Delta x, \Delta y, \Delta z) \) is the maximum cell spacing of the local grid. The definition of \( \Delta \) helps alleviate log layer mismatch in the DDES model.\(^{25}\)

When the DDES length scale \( \ell_{\text{DDES}} \) is equal to the RANS length scale \( \ell_{\text{RANS}} \), the \( k \)-equation returns to its RANS mode. When \( \ell_{\text{DDES}} \) is equal to the LES length scale \( \ell_{\text{LES}} \), the \( k \)-equation will return to a one equation eddy model in LES which is written as

\[ \frac{Dk}{Dt} = 2C_k \sqrt{k} \Delta |S|^2 - C_\epsilon \frac{\sqrt{k^3}}{\Delta} + \nabla [(\nu + \nu_T) \nabla k] \]  \hspace{1cm} (13)

where \( C_k \) is 0.094 and \( C_\epsilon \) is 1.048. To mimic the one equation eddy model in LES, \( C_{\text{DES}} \) is chosen to be 0.95 so that the dissipation part in the DDES model is the same as the one equation eddy model. To make sure the DDES model has the same turbulent production as LES, the turbulent eddy viscosity \( \nu_T \) is rewritten as

\[ \nu_T = (1 - \Phi) \alpha \frac{k}{\omega} + \Phi C_k \sqrt{k} \Delta \]  \hspace{1cm} (14)

where \( \Phi \) is the index showing the region of the LES mode and is defined as

\[ \Phi = \frac{\ell_{\text{RANS}} - \ell_{\text{DDES}}}{\ell_{\text{RANS}} - \ell_{\text{LES}}} \]  \hspace{1cm} (15)

\( \sigma_k \) can be rewritten as \( \sigma_k^* \) so that the diffusion part of \( k \)-equation will be equal to the one
equation eddy model as well.

\[ \sigma_k^* = (1 - \Phi)\sigma_k + \Phi \]  

Unlike previous DDES models that mimic the Smagorinsky subgrid model in their LES parts, a one equation eddy model is used in the LES mode of the new DDES model. The main advantages of this change are that the k-equation is consistently used in the DDES model and the assumption about local equilibrium of energy transfer used in deriving the Smagorinsky model can be dropped.

In the original low Reynolds number correction, \( Re_T \) is defined as \( k/(\omega \nu) \) and only represents the modelled part of turbulence. In the new DDES model, the k-equation is also used to model sub-grid kinetic energy. As a result, the original definition of \( Re_T \) would give a value representing a sub-grid turbulence level that is not applicable for the low Reynolds number correction of the k-\( \omega \) model. Thus, when combining both the low Reynolds number correction and DDES approaches, the definition of \( Re_T \) must be modified to include both the resolved and modelled parts of the turbulence. The new definition of \( Re_T \) should provide a more accurate estimation of the local turbulence level. One way this can be done is to include the resolved turbulent kinetic energy into \( Re_T \). However, estimation of the resolved turbulent kinetic energy requires a time average of the flow field, making the instantaneous simulation depend on historic results. This will make the entire simulation unstable.

In the new DDES model the total turbulent dissipation rate \( \epsilon \) is used to estimate \( Re_T \).

\[ Re_T = \frac{\epsilon}{\omega^2 \nu}, \epsilon = 2(C_{DES} h_{max})^2 \omega |S|^2 + k\omega \]  

The first part of \( \epsilon \) is an estimation of dissipation rate in the LES mode based on the Smagorinsky model. A similar equation has been used in other studies to estimate \( \epsilon \).\textsuperscript{26,27} The second part of \( \epsilon \) is the modelled part. When the turbulent dissipation rate consists only of the modelled component, the new \( Re_T \) reduces to its original definition.

The DDES model was implemented into the open-source computational fluid dynam-
ics (CFD) code OpenFOAM. In the simulations that follow, a second-order, backward-difference method was used for time discretization. Gaussian finite volume integration with central differencing for interpolation was selected for spatial discretization. The Sweeby limiter was used in the convection terms of the k and ω equations. The equivalent of the Rhie & Chow scheme was applied in the divergence term for velocity to remove two-delta waves in the laminar region of transition simulations. Gradients, divergence, and Laplacians are all second-order accurate. The generalized geometric-algebraic multi-grid solver is used as the linear system solver for the pressure equation and the Gauss-Seidel algorithm is used for other variables including velocity, k and ω. The solution for the system of partial conservation equations was obtained, at each time-step, by solving iteratively to a specified tolerance of the residual norm.

Results and Discussion

Transitional Flow in the Micro-scale MIVR

In this section, the new DDES model is used to simulate flow in the micro-scale MIVR. The geometry of the micro-scale MIVR is the same as that in the experimental study of Shi et al. In that experimental investigation, microscopic particle image velocimetry (micro-PIV) was used to measure turbulent velocity fields in the micro-scale MIVR. Three Reynolds number cases were investigated, namely, Re=53, Re=93 and Re=240. where the Reynolds number is defined based on the mean inlet velocity \( U_j \) and the length, \( L \), of one of the sides of the square inlets. Velocity fields at three locations were measured, namely the 1/4, 1/2 and 3/4 planes in the reactor chamber. In the experiments it was found that flow in the micro-scale MIVR is laminar when Re=53. Transition to turbulence begins when Reynolds number increases to 93. Much stronger turbulence appears in the reactor center and outlet at Re=240.

Figure 2 shows the geometry and mesh used in present simulations. In the DDES model,
no refined mesh is needed near the wall as the RANS mode is used there. Note that the ability to apply RANS in the near-wall region is also one of the motivations for applying the DDES approach instead of LES for simulating flow in the micro-scale MIVR. Using the same post-processing technique presented in Liu et al.'s work on the macro-scale MIVR, the velocity fields in the micro-scale MIVR are described in cylindrical coordinates as radial, azimuthal and axial velocities, i.e., $u_r, u_\theta, u_z$. Both experimental and simulation data are averaged along different azimuthal angles within the measurement planes by assuming that the flow within the reactor is axi-symmetric.

All three Reynolds number cases have been simulated by using the new DDES model. Since the model includes the low Reynolds number correction, the new DDES model can be applied to the laminar flow case as well. Thus no switch to the laminar model is required. Figure 3 shows the prediction of mean velocity at $Re=53$ with comparison to experimental data. The radial velocity $u_r$ is well predicted while azimuthal velocity $u_\theta$ is slightly underestimated. It seems that the new DDES model produces excess turbulent viscosity even with the low Reynolds number correction, and this excess viscosity dampens the swirling pattern of flow and underestimates the magnitude of azimuthal velocity. Figure 4 shows the comparison of mean velocity at $Re=93$ between the DDES model and experimental data. The prediction of azimuthal velocity becomes better as the flow begins to transition to turbulence and the DDES model is thus more suitable. The mismatch of radial velocity near the center could be caused by the measurement uncertainty in the experiment because its magnitude becomes very small there. Figure 5 shows the comparison of mean velocity at $Re=240$. A good match between DDES model and experimental data is observed. At $Re=240$, the transition from laminar to turbulence has occurred inside the micro-scale MIVR as evidenced by highly turbulent fluctuations being experimentally observed within the reactor. Previous computational investigations using purely RANS or LES have not accurately modelled the observed turbulence fluctuations. The main disadvantage of applying common RANS models such as the k-ε model to the micro-scale MIVR is in these models, the turbulent in-
tensity is significantly underestimated in the reactor center. Figure 6 presents the prediction of turbulent intensity at Re=240 using the new DDES model, which matches the experimental measurement quite well. Both simulation and experiment confirm that turbulent fluctuations in the MIVR are concentrated near the reactor center. The same phenomenon was also found in the study about the macro-scale MIVR.\(^5\)

**Flow field in the micro-scale MIVR**

The simulation results can be used to investigate how the behavior of the flow changes in the micro-scale MIVR when Reynolds number increases. Streamlines based on mean velocity \(u_r, u_z\) at different Reynolds numbers are shown in Fig. 7. When Reynolds number is increased from 53, to 93, and then to 240, recirculation regions appear and grow in the reactor chamber and move towards the reactor top and bottom. It is also observed that as Reynolds number increases, more flow from the inlet is directed towards the outlet through near the top and bottom surfaces of the reactor. This flow feature potentially hinders the mixing performance of the micro-scale MIVR as flow from different inlets could progress into the outlet near the walls without interaction.

Figure 8 shows the change of the turbulent Reynolds number \(Re_T\) with increasing Reynolds number. \(Re_T\) represents the local turbulence level and depends on the mesh size because only the resolved turbulence level is considered. The discontinuity observed in \(Re_T\) in the center region is a result of mesh refinement there. At Re=53 \(Re_T\) is steady and close to 1 as flow is laminar. Unsteadiness in \(Re_T\) begins to appear in the outlet at Re=93. \(Re_T\) becomes fully turbulent when Reynolds number reaches to 240. This finding is consistent with the experiments of Shi et al.\(^{15}\) The highest levels of \(Re_T\) exists in the outlet of the micro-scale MIVR rather than within the chamber, suggesting that much of the local mixing actually occurs in the outlet region of the micro-scale MIVR.

The mean velocity and turbulent intensity field at Re=240 are further illustrated in Fig. 9. Vertical slices through the reactor are plotted, as the flow is axis-symmetric. In Fig. 9a, it
can also be seen that flow from the inlets enters the outlet primarily near the bottom and top wall area, reinforcing the flow behavior observed in Fig. 7. Figure 9b also indicates that in the middle of chamber most of flow is close to irrotational. $u_z$ (Fig. 9c) is positive everywhere except near the corner regions, indicating that no back flow exists in the reactor center, while back flow is observed when the reactor is scaled up.\(^6\) Note that $u_z$ is much higher than $u_\theta$ in the reactor chamber. However, the magnitude of $u_z$ drops sharply after flow enters the outlet. This is because the swirling flow creates a low pressure zone in the center of outlet, and the resulting adverse pressure grading causes a a decrease in axial velocity. The confined geometry and swirling motion also cause the high turbulence intensity $u'_z$ near the bottom of outlet (Fig. 9f). High turbulent fluctuations in $u'_r$ and $u'_\theta$ are observed in the center of the reactor (Figs. 9d and 9e). However, the observed high turbulence intensity does not necessarily result in enhanced mixing near the center, because unsteady, wandering motion of the vortex center also contributes to the observed fluctuations. The contribution of vortex wandering to turbulence statistics was also discussed in a previous paper by the authors. It is found that 17% - 30% of observed turbulent kinetic energy in the macro-scale MIVR is due to this vortex wandering.\(^5\) If one assumes that turbulence intensity should be isotropic if vortex wandering is not considered, the magnitudes of $u'_r$, $u'_\theta$ should be the same as $u'_z$. Considering their peak values, it is estimated that $u'_r$ and $u'_\theta$ are increased by about 60% near the reactor center because of vortex wandering. This estimation also helps explain the sudden increase of $u'_r$ and $u'_\theta$ at $-0.1 < r/R_0 < 0.1$ in Fig. 6.

**Passive scalar mixing in the micro-scale MIVR**

To further understand how the flow behavior affects the mixing performance of the micro-scale MIVR, passive scalar mixing is studied here. When the turbulence field is correctly predicted, it is relatively easy to model bi-variable passive scalar transport in the reactor.
The governing equation of passive scalar transport can be written as

\[
\frac{\partial \overline{C}}{\partial t} + \frac{\partial (\overline{u}_j \overline{C})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( (D + D_T) \frac{\partial \overline{C}}{\partial x_j} \right)
\]

(18)

where \( \overline{C} \) is the filtered concentration of passive scalar, \( D \) is molecular diffusivity of passive scalar tracer and turbulent diffusivity \( D_T \) is equal to \( \nu_t/Sc_t \). \( Sc_t \) is the turbulent Schmidt number which is usually assumed to be 0.85 in the RANS approach and 0.4 in the LES approach.\(^{31}\) In the new DDES model, \( Sc_t \) is defined as

\[
Sc_t = 0.85(1 - \Phi) + 0.4\Phi
\]

(19)

so that in the DDES model \( Sc_t \) can be 0.85 in its RANS mode and 0.4 in its LES mode.

Passive scalar mixing in the micro-scale MIVR has been previously experimentally measured by using confocal laser scanning microscopy.\(^{32}\) In this experiment, Rhodamine 6G was used as the passive scalar tracer. Two opposing inlet streams contained ethanol, and the other two contain Rhodamine 6G dissolved in ethanol. This configuration is used here in a computational simulation where a zero value of passive scalar represents ethanol and a one hundred value represents the inlet concentration of Rhodamine 6G. The limitedLinear scheme in OpenFOAM is applied to the convection term in equation 19 so that realizable values of passive scalar are ensured.

Figure 10 shows the measured contours of scalar concentration at the 1/2 reactor plane for \( Re=53, 93 \) and 240. The simulation results of the DDES model are shown in Figs. 10a-c and experimental results are shown in Figure 10d-f. The predictions of the transitional DDES model with passive scalar transport agree quite well with experiment where the inner "tai-chi" pattern is reproduced at \( Re=53 \) and 93. As the confocal scanning technique fails to provide a meaningful full field image at \( Re=240 \) due scanning limitations making the time required to generate the full field image to long to effectively "freeze" the flowfield, the instantaneous mixing pattern at \( Re=240 \) can only be revealed by the simulation. It is found
that the inner "tai-chi" collapses at Re=240, although unmixed fluid still exists there. Figure 11 gives a clear view of how the passive scalar mixes in the micro-scale MIVR at Re=53, 93 and 240. Unmixed scalar enters the reactor inner region near the bottom of reactor and then undergoes spiraling motion until diffusion smooths the concentration difference. As Reynolds number increases, turbulent diffusion enhances the mixing of the passive scalar, and the fluid becomes well-mixed when it enters the outlet. Still, there is some unmixed scalar in the reactor chamber, and further increasing the Reynolds number may be required to fully mix the fluid within the reactor.

Conclusions

A new DDES model has been proposed to predict transitional flow in a micro-scale MIVR that has been developed for the manufacturing of functional nanoparticles using the Flash Nanopredictpititation technique. The primary motivation to develop this model is to overcome the difficulty of using RANS approaches in simulating this complex transitional and swirling flow while avoiding the high computational cost of the LES approach. The proposed transitional DDES model is based on the k-ω model with low Reynolds number correction. Through modifying the dissipation rate in the k-equation, the LES mode will be triggered in the simulation domain where the mesh is fine enough. The Low Reynolds number correction in the original k-ω model has also been modified in the transitional DDES model. Both resolved and modeled turbulence are considered in the turbulent Reynolds number $Re_T$ so that the local turbulence level can be estimated more accurately, which can help the switch between RANS and LES.

The transitional DDES model was applied to model the flow at Re=53, 93 and 240 in the micro-scale MIVR, Reynolds numbers that span the laminar and transitional flow regimes. Overall, the simulation results agree quite well with the experimental data collected using microscopic particle image velocimetry in terms of mean velocity and turbulent intensity, thus
validating the accuracy of the proposed transitional DDES model in modeling this complex flow. The simulation results for the micro-scale MIVR also provide a deeper understanding about the flow behavior in the micro-scale MIVR. It is found that flow from different inlets primarily travel through the bottom and top parts of the reactor toward the outlet. By comparing the passive scalar mixing between the simulation and experiment, it is confirmed that the existence of unmixed fluid in the center of the reactor is also caused by this bypass motion of the flow. However, with increasing turbulence level, the amount of unmixed fluid in the reactor can be significantly reduced. Accordingly, the findings in current paper suggest that further optimization of the MIVR is necessary to improve its mixing performance, especially near the bottom of the reactor.

Acknowledgement

The author would like to thank Dr. Paul A. Durbin for the discussion about current simulations and Dr. Yanxiang Shi for providing the experimental data. This research is supported by Grant CBET-0932978 and S12-SSE-1440443 from the National Science Foundation.

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Figure 1: Dependence of $C_\mu$, $\alpha^*$ and $C_{\omega_1}$ on turbulent Reynolds number $Re_T$.

Figure 2: Geometry and mesh of the micro-scale MIVR.
Figure 3: Comparison of normalized mean velocity at Re=53 between DDES and experiment: 
\(\frac{<u_r>}{U_j}\), \(\frac{<u_\theta>}{U_j}\).

Figure 4: Comparison of normalized mean velocity at Re=93 between DDES and experiment: 
\(\frac{<u_r>}{U_j}\), \(\frac{<u_\theta>}{U_j}\).
Figure 5: Comparison of normalized mean velocity at Re=240 between DDES and experiment: a $<u_r>/U_j$, b $<u_\theta>/U_j$.

Figure 6: Comparison of normalized turbulence intensity at Re=240 between DDES and experiment: a $<u'_r>/U_j$, b $<u'_\theta>/U_j$. 
Figure 7: Effect of Reynolds number on mean flow field in the micro-scale MIVR: a Re=53, b Re=93, c Re=240.

Figure 8: Effect of Reynolds number on turbulent Reynolds number $Re_T$: a Re=53, b Re=93, c Re=240.
Figure 9: Mean and turbulent intensity contour at \( \text{Re}=240 \): a \( u_r \), b \( u_\theta \), c \( u_z \), d \( u'_r \), e \( u'_\theta \), f \( u'_z \)
Figure 10: Comparison of passive scalar mixing between DDES (a Re=53, b Re=93 c Re=240) and experiment (d Re=53 e Re=93 f Re=240).
Figure 11: Effect of Reynolds number on passive scalar mixing: a Re=53, b Re=93, c Re=240.
Highlights

- A transitional delayed detached eddy simulation model was developed for use in microscale vortex reactors
- Simulation results were compared to microscopic particle image velocimetry and laser induced fluorescence experiments
- Excellent agreement was observed between simulation and experiment
- The model accurately simulated both the laminar and turbulent flow regimes in the reactor