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NUMERICAL STUDY OF MULTI-COMPONENT FLOW AND MIXING IN A SCALED FISSION PRODUCT VENTING SYSTEM

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Abstract

Numerical simulation of isothermal multi-component gas flow was conducted to study fluid flow and mixing in a scaled low-pressure, low-temperature test facility for the fission product venting system (FPVS) of a gas cooled fast reactor (GFR). The geometry of FPVS test facility was an open loop including gradual expansion coupling and two 90° pipe elbows.

First, the validation of large eddy simulation (LES) wall-adapting local eddy-viscosity (WALE) turbulent model was performed for transitional flow in a circular pipe with gradual expansion. The reactingFOAM solver in OpenFOAM v8 was employed. By introducing appropriate turbulence disturbance at the flow inlet, such as turbulence intensity, the numerical results showed good agreement in (1) the velocity profile downstream of the pipe expansion measured by particle image velocimetry (PIV) in this study, and (2) the reattachment length reported in the literature.

Using this validated model, the numerical simulation of flow and component mixing was performed for the FPVS with an inlet flowrate corresponding to a Reynolds number of 2,400 to investigate the flow behavior and component mixing. Standard deviation of the mass fraction of component, referred to as absolute mixing index (AMI), was calculated to quantify the mixing of compo-

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nents, showing that the component mixing length determined by AMI is related to the reattachment length downstream of the expansion. Finally, this study was able to identify the best location in the FPVS test facility to measure the velocity and concentration profiles where multicomponent flow is well mixed.

Keywords: LES, transition flow, reattachment length, axisymmetric expansion flow, pipe bend flow, mixing

Nomenclature

$\langle X \rangle$	Averaged value of X over a cross section
α	Fraction of new random component added to previous time value
$\dot{m}_i$	mass flow rate at the inlet
$\dot{m}_p$	mass flow rate at the porous wall
$\mathcal{R}$	Equally distributed random variable between -0.5 and 0.5
ν	Kinematic viscosity
$\bar{w}_i(x, y, z)$	Temporally averaged mass fraction of surrogate gas i at a specific point on the cross section
ρ	Density
σ	Standard deviation
A	Cross-sectional area
C_{rms}	RMS coefficient, $\sqrt{12(2\alpha - \alpha^2)}/\alpha$
I	Turbulence intensity
U_b	Bulk velocity
U_{inlet}	Inlet velocity of current time step
U_{old}	Inlet velocity of previous time step
U_{ref}	Reference velocity
θ	Angle of expansion
D	Diameter of the large pipe
d	Diameter of the small pipe
h	Step height

Lr	Reattachment Length
Re	Reynolds number DU_b/ν
R	Radius of a pipe
r	Radial location
AMI	Absolute Mixing Index
CL	Cartridge Loop
CR	Curvature Ratio
DNS	Direct Numerical Simulation
ER	Expansion Ratio
FPVS	Fission Product Venting System
GFR	Gas Cooled Fast Reactor
LES	Large Eddy Simulation
LPLT	Low Pressure Low Temperature
TI	Turbulence Intensity
VTR	Versatile Test Reactor

1. Introduction

Texas A&M University is participating in the Versatile Test Reactor (VTR) project by the Department of Energy (US DOE) to study the transport of gaseous fission products in the fission product venting system (FPVS) test facility of the Gas Fast Reactor Cartridge Loop (GFR-CL). The VTR programs aim to incorporate multiple cartridge loops, each operating with different coolants (i.e., liquid metal, molten salt, sodium, and helium) to accelerate the testing of advanced nuclear fuels, materials, coolants, instrumentation, and controls. Several industry partners, such as General Atomics (GA), have invested in advanced nuclear reactor technology. The Energy Multiplier Module (EM2) is a conceptual design by GA for a helium-cooled fast reactor. Therefore, the helium-cooled CL is a candidate for testing in the VTR facility that will aid the design and construction of gas-cooled reactors in future.

The FPVS is designed to extract and transport an adequate amount of fission products produced in the GFR-CL, comprising the primary coolant in a circular cross-section loop along with fission gases such as xenon, krypton, and iodine, and similar fluids that flow through the FPVS loop. The transport phenomena inside the FPVS are quite complex because of the mixing of multicomponent fluids, which flow through curved sections at high pressures and temperatures. The flow within the FPVS can vary from laminar to turbulent. Heat generation in the reactor might induces a temperature gradient within the loop. Curved sections in the loop generate Dean flows, re-laminarization, and swirl-switching phenomena.

The GFR-CL and its FPVS are operated under high pressure and high temperature, with helium as the primary coolant or medium. The expected fission products are xenon, cesium, krypton, iodine, etc. Under accident conditions, the fission products might include solid particulates. These operating conditions and materials cannot be replicated in a university laboratory environment owing to safety considerations. Thus, we performed scaling analysis. Air was identified as the primary coolant, and argon and carbon dioxide were identified

as surrogate fission product gases. Thus, a low-pressure low-temperature (atmospheric conditions) transparent facility was constructed following a scaling exercise. The transparent loop was operated under standard atmospheric temperature and pressure conditions. Air was used as a surrogate primary coolant
 35 in lieu of helium and argon was used as a surrogate fission product gas. Other conditions, such as the flowrate, were modified based on similitude.

The numerical simulation conducted in this study was focused on a low-pressure low-temperature transparent experimental test facility. There were two distinctive geometries in the loop that impacted the flow and mixing of the
 40 primary surrogate coolant and surrogate fission product gases. These included a pipe expansion where the diameter of the pipe was increased with a pipe coupling and an elbow.

The geometry of sudden/gradual expansion is one of interesting aspects with respect to mixing because thermal and component mixing in the pipe flow is
 45 almost completed by localized turbulence observed downstream of the sudden expansion. Flow recirculation occurs at the corner of the expansion. This recirculation region can be described by the reattachment length L_r , defined as the length between the expansion and the point at which the direction of the axial velocity in the vicinity of the wall is reversed. In the laminar region, the
 50 reattachment length is directly proportional to the Reynolds number. Results from both dye injection experiments by both Latornell & Pollard (1986) and Pak et al. (1990) as well as from DNS by Moallemi & Brinkerhoff (2018) show a linear correlation of $Re/h = 0.0885L_r$ for flow through a pipe with an expansion ratio of 2. Re is the upstream Reynolds number defined as Ud/ν and h is a
 55 step height of the pipe expansion. The expansion ratio is defined as the ratio between the two different pipe diameters in the expansion flow.

At higher Reynolds numbers in the transition region, the reattachment length decreases with an increase in the Reynolds number. The stratified flow becomes unstable and collapses at a distance shorter than that in laminar flow
 60 due to localized turbulence. Several efforts have been made to measure this threshold value. Selvam et al. (2015) conducted numerical simulation for grad-

ual expansion. For Re is 1,680 or higher, with this level of disturbance as
 mentioned above, localized turbulence was triggered. Mullin et al. (2009) mea-
 sured the velocity profile using magnetic resonance imaging (MRI) and found
 65 the critical Reynolds number to be 1,139. Below the critical Reynolds number,
 the asymmetry of velocity profiles increased as the Reynolds number increased
 while a constant low asymmetry was observed below the critical Reynolds num-
 ber. Furuichi et al. (2003) measured the axial velocity using an ultrasound
 technique, and the velocity profiles suggested that the critical Reynolds number
 70 was 1,500. The ambiguity in the value of the critical Reynolds number was
 due to the complexity of the expansion flow in the transition region. Sreeni-
 vasan & Strykowski (1983) studied the flow through expansion using a hot wire
 anemometer. They observed fluctuations and oscillations in the flow down-
 stream of the expansion. The same observations were made by Furuichi et al.
 75 (2003) using an ultrasound technique and Mullin et al. (2009) through MRI.
 In addition, the reattachment length can be altered by the shape of the inlet
 flow profile, amount of disturbance, or turbulence intensity. Latornell & Pollard
 (1986) conducted a dye injection experiment for a circular pipe and concluded
 that the reattachment length depends on the shape of the inlet profile. The
 80 reattachment length with a plug profile at the inlet (high Turbulent kinetic en-
 ergy (TKE)) is shorter than that with a fully developed profile used at the inlet.
 Sanmiguel-Rojas & Mullin (2012) and Selvam et al. (2015) showed that a small
 flow perturbation perpendicular to the main flow impacts both the magnitude
 and location of the onset of instability. Ngyuen et al. (2019) introduced vortex
 85 perturbation for DNS of a sudden expansion flow and showed that the critical
 amplitude or vertex perturbation is proportional to Re^{-3} . Vittal Shenoy et al.
 (2020) studied flow through a gradual expansion and the critical amplitude was
 found to be proportional from $Re^{-2.1}$ to $Re^{-4.6}$ for a gradual angle θ from 45°
 to 4.76° , respectively.

90 Generally, downstream of the transition region, there exists a turbulent re-
 gion in which the reattachment length is no longer dependent on the Reynolds
 number. Pak et al. (1990) also conducted dye injection experiments with ex-

pansion ratios of 2 and 2.667. Milk diluted with alcohol and water mixture were injected into the water flow. The reattachment length remained constant
 95 at $Re > 3,000$. Sanmiguel-Rojas et al. (2010) explained this using global mode analysis for a sudden expansion flow with an expansion ratio of 2. The flow became linearly unstable at a critical Reynolds number of 3,273 or higher, and it corresponded to a oscillatory bifurcation with wave number $|m| = 1$ located at the end of the recirculation region. This implies that localized turbulence
 100 was generated regardless of the inlet condition.

It is interesting that localized turbulence can be generated even in the laminar region of a circular pipe flow with a Reynolds number below 2,100. This implies that laminar and turbulent flows can coexist in pipe expansion flows, thus preventing the use of conventional RANS-based turbulence models to simulate the flow. Hence, either LES or DNS approaches are required to simulate
 105 flows through the expansion geometry in the scaled FPVS test facility. Numerical simulation for the scaled FPVS test facility built at Texas A&M University has to consider it because expected operating conditions of the facility is ranged Reynolds number of 1,000 to 5,000.

Flow through 90° pipe bend is another interesting flow behavior with respect
 110 to mixing. Experimental measurement of velocity fields through 90° pipe bends flow with Reynolds number (Re) of 6×10^4 and Curvature ratio (CR) of 2.0 was performed by Sudo et al. (1998), showing that high axial velocity was observed at inner wall of the bend at 30° angle, and it was shifted to the outer wall of the bend downstream of the 90° pipe bend. Secondary flow and biased axial
 115 velocity distribution toward outer wall of the bend was remained even up to 10 downstream of the bend exit. Flow separation and reattachment flow were observed in the elbows. Numerical simulation with $k - \epsilon$ model conducted Dutta et al. (2016) and Dutta & Nandi (2019) showed that for Re of 1×10^5 ,
 120 the separation angle was found to be 61°, 73° and 88.8° for CR of 0.75, 1.0 and 1.25, respectively, and the reattachment point was observed to be 0.05D $\sim$ 0.31D downstream of the 90° elbow. Rütten et al. (2005) performed large eddy simulation (LES) of flow through a 90° pipe bend for Re of 5,000, 10,000

and 27,000 and CR of 1.0 and 3.0, reporting that flow separation was observed
125 at the bend geometry with CR of 1.0 while no separation was found at the
bend geometry with CR of 3.0. Also, a pair counter-rotating Dean vortices was
observed in the pipe bend flow and the size and axis of each vortex was switching
continuously, referred to as the swirl switching phenomena. The review paper
written by Kalpakli Vester et al. (2016) described it in detail. Carlsson et al.
130 (2015) studied that very-large-scale motions(VLSMs) is related to switching in
pipe bend flow by performing proper orthogonal decomposition (POD) analysis
by the mean of LES for the geometry with $Re=34,000$ $CR=1\sim1.67$. There are
some direct numerical simulation (DNS) flows through 90° pipe bend. Noorani
et al. (2013) performed DNS for 90° pipe bend at moderate Re of 5,300 and
135 11,700 and curvature ratio of (CR) of 5. Hufnagel et al. (2018) studied swirl-
switching in pipe bend flow for Re of 11,700 and CR of 1.67 using 3D POD
analysis with DNS.

The objective of this study is to investigate the mixing in the FPVS test
facility, numerically. There are some challenges. First, pipe flow with moderate
140 Reynolds number number (1,000~5,000) estimated by the mean of numerical
simulation is unclear so far. It is expected that flow separation and reattachment
observed downstream of the expansion and downstream of pipe bend can affect
mixing in the pipe flow because separated recirculation layer might attenuate
the mixing. Furthermore, strong localized turbulence induced downstream of
145 the expansion can enhance the mixing. However, only a few numerical studies
try to estimate reattachment length for transition flow in a sudden/gradual
expansion flow numerically, but faced these challenges. Moallemi & Brinkerhoff
(2018) estimated the reattachment length for the sudden expansion flow as a
function of Reynolds number using the DNS but their result is overestimated
150 compared with other experimental reference in the transition region. Ngyuen
et al. (2019) and Vittal Shenoy et al. (2020) studied characteristics of flow
through sudden/gradual expansion as a function of turbulence disturbance at
the inlet but they did not estimate the reattachment length. In addition, DNS
requires enormous a lot of computational resource and thus is not good for

155 parametric studies. Secondly, there is no universal value to quantify the mixing
of multicomponent flow in the pipe.

In this study, the validation of LES model to estimate the reattachment
length numerically for expansion flows is performed. The solver *reactingFoam*
with the LES wall-adapting local eddy-viscosity (WALE) model in OpenFOAM
160 v8 was selected for the CFD simulation. To validate the model, axial velocity
profile calculated from the numerical simulation is compared with particle im-
age velocimetry (PIV) measurement in the scaled FPVS test facility and the
numerically calculated reattachment length estimated is compared with data
reported in the literature. It is revealed that turbulent disturbance at the inlet
165 flow is the key factor in estimating the reattachment length in flow through the
expansion.

With validated model, multi-component CFD simulation was performed for
FPVS test facility with Re of 2,400, ER of 1.5, and CR of 4.0. The flow char-
acteristics and mixing behavior in a scaled FPVS test facility and the identifi-
170 cation of best locations for measuring velocity and concentration for sampling.
The concept of absolute mixing index (AMI) was introduced to quantify the
component mixing at each cross-section as a function of axial distance. The
parametric study for the flowrate at the porous wall showed that the mixing
length determined by AMI is related to the reattachment length of flow through
175 the expansion flow.

2. Experimental and Numerical Setup

2.1. Geometric configuration and scaling

The system discussed in this paper is shown in Figure 1-(a), referred to as
low pressure low temperature (LPLT) FPVS test facility because it operates at
180 atmospheric pressure and temperature. The geometry of the domain to mimic
the LPLT FPVS test facility is shown in Figure 1-(b). The LPLT FPVS test
facility has a U-type loop and operates in an open-loop mode. During the open-
loop test, the scaled high-temperature absorber (HTA) part shown on the left

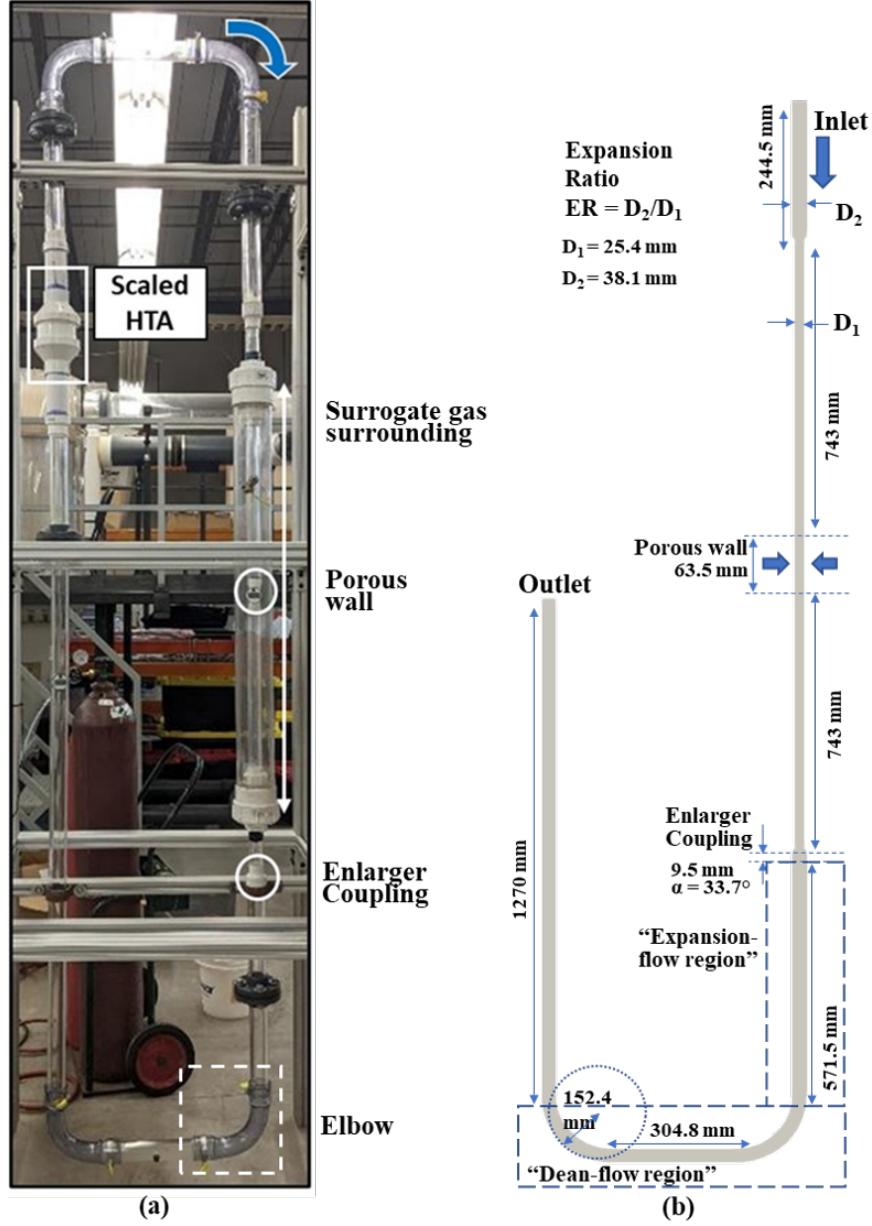


Figure 1: (a) Low-temperature, low-pressure experimental facility, (b) Schematic geometry used in the numerical simulation

of Figure 1 is disassembled from the facility. Coolant gas is introduced at the
 185 “inlet” and surrogate gas is injected into the loop through the porous wall from
 the ambient surrogate gas surrounding to simulate the flow through GFR CL.
 The porous wall lies in the middle part of the thin pipe with a length of 76.2 mm.
 The region surrounding the porous tube was not simulated but was specified as
 a boundary condition in this study.

190 This loop is comprised of two different sizes of pipe, with inner diameters
 of 25.4 mm and 38.1 mm, respectively. Expansion ratio ($ER = d/D$) is 1.5. A
 part connecting two pipes of different diameters is called a reducer or enlarger
 coupling. The region downstream of the enlarger coupling from a thin pipe to
 a thick pipe is of interest and named as “expansion-flow region” in this study.
 195 Similarly, Dean flows occur at the pipe bend is of interest in this study as it
 impacts mixing, too. The “Dean-flow region” is comprised of two 90 degree
 elbows and connecting straight pipe between each elbow. Curvature ratio (CR
 $= R_c/D$) of each elbow is 4 in this study, where R_c is radius of curvature of the
 loop, D is diameter of the pipe.

200 The surrogate fluids were chosen based on scaling performed to simulate the
 mixing of helium coolant and fission gas that occurs in the FPVS. Dimensionless
 parameters, such as the Froude, Schmidt, Richardson, and Reynolds numbers,
 which govern the thermal-fluid dynamics of the studied phenomena were applied
 in the scaling. The Thermal-fluid dynamics similarity of the experimental facil-
 205 ity and cartridge loop was obtained by imposing the ratio of the dimensionless
 numbers equal to unity. The similarity of the Froude, Richardson, and Reynolds
 numbers are related to length, temperature, and velocity scaling, respectively.
 The Schmidt number similarity is related to the thermal-fluid properties of he-
 lium and air. To guarantee the thermal-fluid dynamics similarity of the model
 210 to the prototype, the ratio of the dimensionless numbers was set to unity:

$$\Psi_R = \frac{\Psi(model)}{\Psi(prototype)} = \frac{\Psi_m}{\Psi_p} = 1 \quad (1)$$

where subscripts m, p and R denote the “model”, “prototype”, and their ratio,
 respectively. Through algebraic manipulation, Reynolds and Froude numbers

give the velocity of the working fluid as a function of the properties of both the model and prototype and the prototypical velocity.

$$U_m = \sqrt[3]{\frac{\nu_m}{\nu_p} \frac{\rho'_m}{\rho'_p} U_p^3} \quad (2)$$

215 where ν is the kinematic viscosity, $\rho' = \frac{\rho_{coolant} - \rho_{fission\ gas}}{\rho_{coolant}}$, and ρ is the density. The fluids were assumed to be under isothermal conditions. The porous region was scaled to one-to-one ($L_m/L_p = 1$) and the high temperature absorber (HTA) has a scaling of 1 to 23 ($L_m/L_p = 1/23$). The rest of the geometric parameters were established to accommodate required flowrate.

220 The temperature and pressure for LPLT FPVS test facility were specified as room temperature 300 K and atmospheric pressure, respectively. From this similitude analysis, the primary and secondary surrogate gases were identified as air and argon, respectively. For this study, the inlet velocity in the test facility was determined to be 1 m/s and 0.002856 m/s at the porous wall.

2.2. Numerical setup

Time-dependent multicomponent fluid simulation was conducted using OpenFOAM v8, an open-source CFD simulation program. The *ReactingFOAM* solver was employed. This is a *pimpleFOAM*-based multicomponent variant-density flow solver. The time step was specified as between 1×10^{-4} and 1×10^{-3} 230 seconds, not to exceed Courant-Friedrichs-Lewy (CFL) value of 3 during the simulation run. The *PimpleFOAM* iteration settings, nOuterCorrectors, nCorrectors and nNonOrthogonalCorrectors were set as 5, 2 and 1, respectively. Convergence at each time-step is achieved when the residual of each property was less than 1×10^{-5} except for 1×10^{-6} in the final loop. A second-order backward 235 difference scheme was used to calculate the temporal derivative. The LUST scheme was used to calculate the spatial derivative of velocity, and the second-order central difference scheme was used to compute other spatial derivatives. Simulation runs were made for 20 seconds, and the temporally averaged velocity and turbulence quantities were calculated. Information achieved during the first 240 5 seconds was excluded from the calculation of the average of properties.

We adopted LES with the WALE model proposed by Nicoud & Ducros (1999), which can be used from the laminar to turbulent region for anisotropic flow. Li et al. (2019) conducted LES with a WALE model to reproduce the turbulence flows of twin parallel jets and observed good agreement with PIV measurements. In addition, The LES model was compared with the PIV measurements made in the LPLT FPVS test facility and found to agree well. This is explained in detail in the next section. Therefore, The WALE LES model was selected as the turbulence model in this study. The velocity profile of the fully developed laminar flow in the circular pipe was used for the inlet velocity condition. To initiate the turbulence in the pipe flow, a random fluctuation in velocity was introduced at the pipe inlet and a normal component of velocity was introduced at the inlet (0.1~1% of the axial velocity). The built-in boundary condition *turbulentInlet* of the OpenFOAM v8 is employed as a inlet boundary condition. The velocity equation at the inlet is written as:

$$U_{inlet} = (1 - \alpha)U_{old} + \alpha(U_{ref} + C_{rms}|U_{ref}|I\mathcal{R}) \quad (3)$$

$$U_{ref} = \delta U_b \mathbf{e}_x + 0 \mathbf{e}_y + U_b \mathbf{e}_z \quad (4)$$

where U_{inlet} is the velocity at the inlet, U_{old} is the inlet velocity of previous time step, U_{ref} is the reference velocity, $|U_{ref}|$ is the magnitude of the reference velocity, δ is the fraction of flow disturbance compared with mainstream flow, α is the fraction of new random component added to previous time value, C_{rms} is the RMS coefficient, the z coordinate is the axial direction, r is the radial location, R is the radius of pipe, U_b is the mean velocity, I is the turbulence intensity and $\mathcal{R}$ is an equally distributed random variable between -0.5 and 0.5.

The reattachment length is defined as the length between the end of gradual expansion to the reattachment point where the flow adjacent to the wall reverses. Temporally averaged axial velocity is employed to calculate the reattachment length.

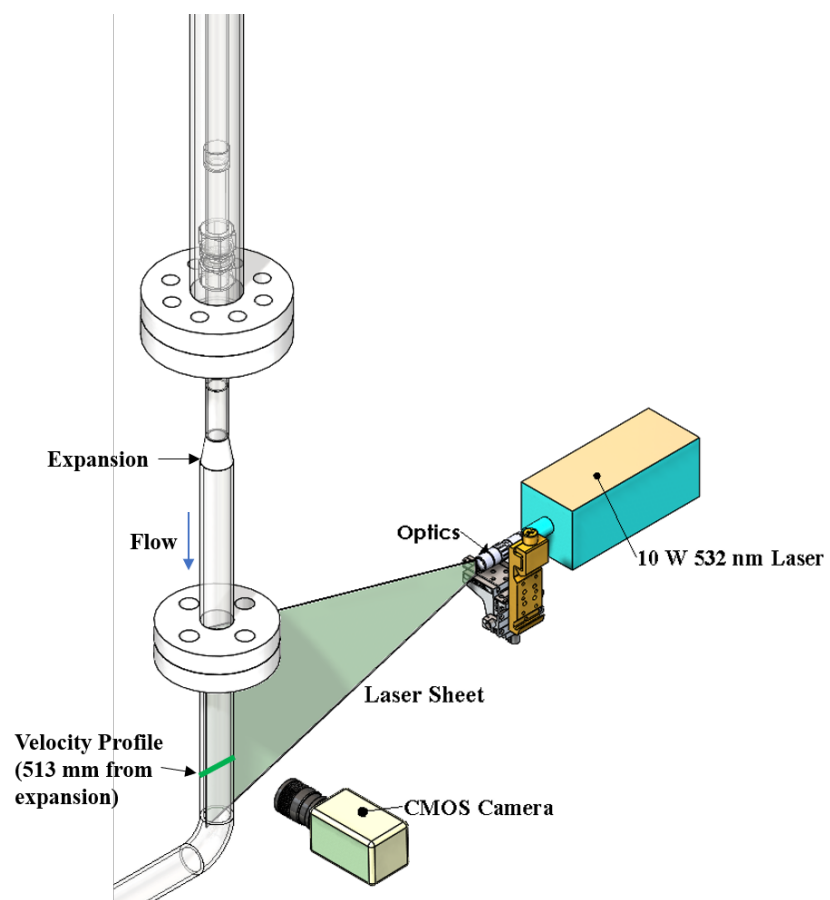


Figure 2: Particle image velocimetry (PIV) experimental setup in the LPLT facility.

2.3. Experimental measurement technique

The basic working principle behind Particle Image Velocimetry (PIV) measurement technique deals with quantifying the pixel displacement of the seeding particles in the fluid for sequential images. An instantaneous velocity vector can be calculated by estimating the pixel displacement between consecutive images. The main components to perform the measurement technique include reflective seeding particles, a light source, optical instruments, and a camera. In this study, a 10 W monochromatic continuous laser of a visible wavelength of 532 nm is employed along with a CMOS Phantom M310 camera. The laser paired with a collimator and optical lenses (TSI 610026) illuminates the seeding particles and reflected light is captured by the camera sensor to create images. Both the laser head and the camera were mounted on separate motorized-traverses to adjust the positioning. Figure 2 shows the facility used for carrying out an experimental measurement using the PIV technique. The LPLT experimental facility was designed to simulate pressure driven flow in GA's EM² FPVS system. The facility is constructed of clear acrylic plastic to aid flow visualization techniques. The coolant gas was mixed with smoke particulates in a chamber prior to injection at the inlet. Air was injected at 1 m/s and verified using a hot-wire anemometer. An average 2-D velocity plane was calculated over a period of 3 seconds (3,000 frames). From the 2-D plane, a line velocity profile was used for numerical comparison. The locations of the line profiles are shown in Figure 2.

2.4. Experimental uncertainty

The collected 12-bit depth images were processed by multi-pass, multi-grid, PIV algorithms commonly referred to as PRANA that employs robust phase correlations RPC Eckstein & Vlachos (2009b). A three-step process was applied. The initial interrogation window was a 64 x 64 pixel area, followed by two interrogation areas of 32 x 32 pixels. All passes had a window overlap of 50% . The PIV measurement had 50 x 80 instantaneous velocity vectors. Cross-correlations were executed by RPC algorithm, which reduces errors in the

presence of high rotational motion compared to standard algorithms Eckstein & Vlachos (2009a). Universal outlier detection approach proposed by Westerweel (1994) was applied to determine spurious vectors and replaced via interpolation. The spurious and erroneous vectors for the velocity were evaluated to be less than 1.5%. The study of Timmins et al. (2012) estimated the uncertainty of PRANA to be approximately 0.1 pixels. The PIV uncertainty propagation discussed in Sciacchitano (2019) was estimated for the statistical results and uncertainty associated with the velocity was estimated to be less than 2% based on the methods applied in Sciacchitano (2019), which agrees well with previous literature such as the works of Hyun et al. (2003) and Elahi et al. (2017).

3. Validation of Numerical Model

3.1. Grid Convergence Test

Grid convergence test has been performed with simplified geometry of gradual expansion flow as illustrated in Figure 3. First, The cross-sectional mesh varied from non-uniformly sized 405 to 1,280 cells, with constant axial direction mesh size of 3 mm. On finest mesh, the cell sizes in the vicinity of the wall are 8.414×10^{-5} m and 3.008×10^{-4} m for small and large diameter pipe, respectively, which were of the order of y^+ for given Reynolds number of 3,591 based on small diameter pipe. The grid independence for this step was established by monitoring the grid convergence index (GCI) suggested by Roache (1994), defined as $GCI = F_s \epsilon / (r^p - 1)$ where F_s is safety factor of 1.25, $\epsilon = (f_1 - f_2) / f_1$ is relative error, r is grid ratio and p is order of method. The reattachment length is chosen as f_1 , f_2 and f_3 for each mesh, respectively. Grid independence was declared when the GCI ceased to vary by more than 1% (Table 1). To establish overall grid independence, the cross-sectional mesh size (number of cells) was maintained constant at 1,280 and applied to the geometry shown in Figure 1-(b). The axial height of the mesh size was varied from 2.822 mm to 9.474 mm such that the total number of cells varied from 0.66 million to 2.23 million. The reattachment length downstream of the expansion was calculated, and the

results are listed in Table 2. The error was defined in relation to the adjacent case with a sparse mesh. With an axial cell height of 3.449 mm or less, the calculated error was reduced within 1%. Accordingly, grid independence was declared with an axial cell height of 3 mm. All simulation runs were performed in this study with an cross-sectional mesh of 1,280 cells and an axial mesh size of 3 mm.

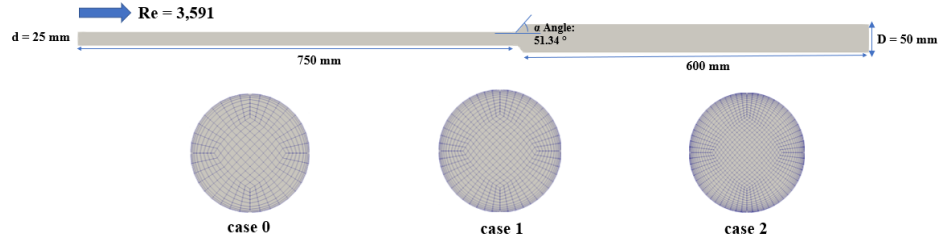


Figure 3: Geometry and mesh used for grid independence

Table 1: Grid convergence index with different cross-sectional mesh

Case	Expansion Ratio	Number of Cells in a Cross-Section	Number of Cells	Reattachment Length [m]	Order of convergence: p	Grid Convergence Index (GCI)
ER1.8_case0	1.8	405	183,870	0.2511		
ER1.8_case1	1.8	720	326,880	0.2843	9.1760	1.119%
ER1.8_case2	1.8	1,280	581,120	0.2866	9.1760	0.079%
ER2.0_case0	2.0	405	183,870	0.2769		
ER2.0_case1	2.0	720	326,880	0.3034	5.5240	2.79%
ER2.0_case2	2.0	1,280	581,120	0.3088	5.5240	0.56%

Table 2: Grid independence test with different axial cell height

Case	Expansion Ratio	Number of Cells in a Cross-Section	Axial Cell Height [mm]	Number of Cells	Reattachment Length [m]	Error [%]
Axial Case 1	1.5	1,280	9.474	665,600	0.3013	-
Axial Case 2	1.5	1,280	6.350	990,720	0.3465	13.06
Axial Case 3	1.5	1,280	4.233	1,486,080	0.3316	4.51
Axial Case 4	1.5	1,280	3.449	1,825,280	0.3299	0.52
Axial Case 5	1.5	1,280	2.822	2,232,320	0.3328	0.87
Axial Case 6	1.5	1,280	2.300	2,736,640	0.32999	0.84

3.2. Comparison with PIV measurements

A flow visualization experiment was conducted in the LPLT FPVS test facility to validate the numerical model. Air was injected at the inlet without any

335 injection through the porous wall. The bulk velocity at the inlet was measured
 using a hot-wire anemometer and controlled approximately 1 m/s, correspond-
 ing to a Reynolds number of 2,394 at the inlet (equivalent to Re of 3,591 based
 on small diameter pipe). The PIV measurements were made at 0.513 m down-
 stream of the expansion in the “expansion-flow-region”. See the location on
 340 Figure 4-(a). Accurate measurement of turbulence intensity at the inlet is not
 available, so LES calculation is made with 5, 10, 15, and 20% turbulence in-
 tensity values and compared with PIV measurements. Figure 4-(b) shows the
 axial velocity profiles over radial direction (or x-coordinate direction) measured
 by PIV and estimated by LES. Green line with circle mark represents axial
 345 velocity profile by the PIV measurement, and straight lines does for the nu-
 merical simulation with four LES with different turbulence intensity (5, 10, 15,
 and 20%) at the inlet. Table 3 represents the maximum and bulk velocity and
 the associated relative percent difference compared to the PIV measurement at
 the location seen on Figure 4-(a). The bulk velocity is calculated by taking
 350 the surface integral of the velocity profile and both the PIV measurements and
 LES calculations yield bulk velocity of 1 m/s, similar to the measurement made
 by the anemometer at the inlet. The LES result shows axial velocity profiles
 and its maximum velocity are sensitive to turbulence intensity. Maximum axial
 velocity from LES result with turbulence intensity of 5% has 92.48% difference
 355 compared to PIV measurement while that with turbulence intensity of 20% does
 3.06% difference. We can conclude that PIV measurement and LES simulation
 result with turbulence intensity of 20% are in good agreement. In conclusion,
 the LES with the WALE model has good agreement with the experimental
 measurements downstream of “expansion-flow-region” with assumed value of
 360 turbulence intensity of 20%.

3.3. Comparison with reference data in terms of Reynolds number

The reattachment length was selected to quantify the mixing of the flow
 downstream of the expansion joint. The inlet flowrate was varied such that the
 Reynolds number varied from 500 to 6,000. This parametric runs for gradual

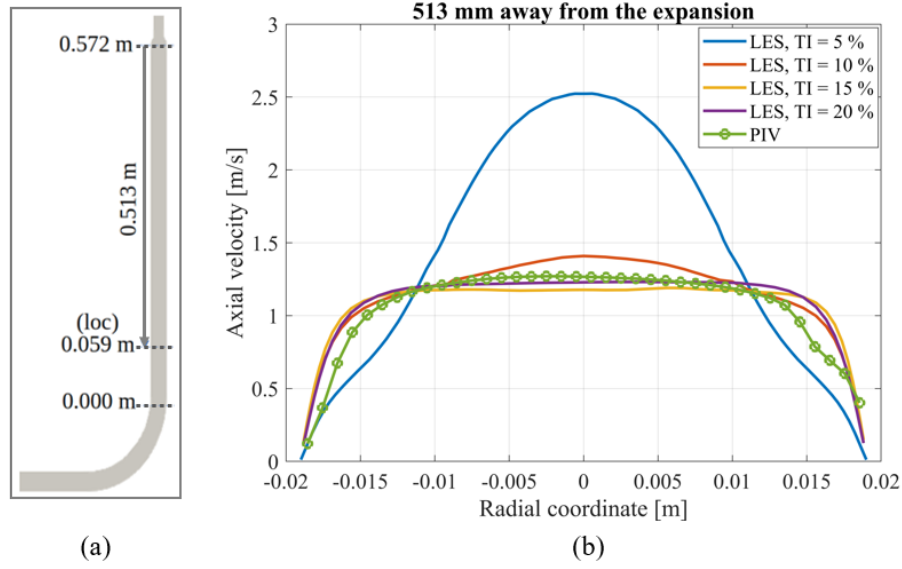


Figure 4: Axial velocity profile downstream of the expansion

Table 3: Comparison between PIV measurement and LES result

Location	0.513 m away from the expansion				
Method	PIV	LES	LES	LES	LES
Turbulence Intensity		T =5%	TI=10%	TI=15%	TI=20%
Bulk velocity [m/s]	1.0382±0.0208	1.0031	1.0037	1.0017	1.0023
Difference [%]	-	3.3804	3.3214	3.5109	3.4605
Max velocity [m/s]	1.2704±0.0254	2.4452	1.4091	1.19	1.2315
Difference [%]	-	92.4835	10.9194	6.3243	3.0584

365 expansion flow were made by introducing both flow disturbance perpendicular
 to axial velocity and specifying the turbulence intensity at the inlet. The flow
 disturbance in the perpendicular direction to the mainstream flow at the inlet
 was set at 1% of the mainstream flow velocity and the inlet turbulence intensity
 was set a high value of 60%. The Reynolds number calculation was based on
 370 flow with a smaller diameter pipe. The reattachment length was estimated for a
 sudden expansion flow with an expansion ratio of 2. In Figure 5, It is observed
 that our result is in good agreement with measurements made by Latornell &
 Pollard (1986) and Pak et al. (1990) using a dye injection method. Consistent
 with the findings of Furuichi et al. (2003), we observe three distinct regions in
 375 the calculation of the reattachment length as a function of the Reynolds number
 in current CFD simulation study. In the laminar region ($Re = 500-1,000$), the
 reattachment length normalized to the step height is linearly proportional to the
 Reynolds number (Figure 5). In the turbulent region (expected above 3,500),
 the normalized reattachment length is independent of the Reynolds number
 380 and becomes constant. In the transition region located between the laminar
 and the turbulent regions, the reattachment length tends to rapidly decrease
 as the Reynolds number increases. Although the qualitative variation in the
 CFD simulated value of the normalized reattachment length is consistent with
 the results reported in literature (Latornell & Pollard (1986), Pak et al. (1990),
 385 and Moallemi & Brinkerhoff (2018)), there is no quantitative agreement on the
 transition region. The quantitative disagreement between the current CFD sim-
 ulations and the values reported in literature can be attributed to the impact
 of turbulence intensity at the inlet on the reattachment length in the transition
 region. A higher flow disturbance can help to cause Kelvin-Helmholtz insta-
 390 bility downstream of the expansion due to the velocity difference between two
 layers, resulting in shorter reattachment lengths. The higher the turbulence
 intensity is, the shorter the reattachment length is. The turbulence intensity
 at the inlet affects not only the reattachment length but also the location at
 which the reattachment length starts to decrease with increase in the Reynolds
 395 number. Based on this explanation, we can expect that the flow disturbance

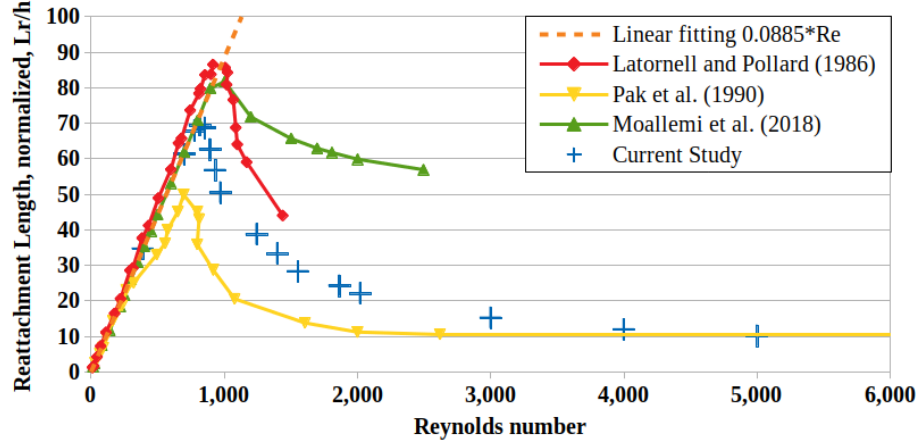


Figure 5: Comparison with reference data with different Reynolds number

and turbulence intensity at the expansion in the study of Pak et al. (1990) is higher than that in the current study, while that of Latornell & Pollard (1986) is lower than that in the current study. Considering this, the CFD solver and turbulence model chosen for the current study are hereby validated. Note the
400 turbulence intensity at the expansion is smaller than that of inlet as turbulence energy is dissipated in laminar flow.

4. Results and Discussion

CFD simulations were conducted for multicomponent gas flow in the LPLT FPVS test facility to study the mixing of air and argon. The primary flow
405 including air and argon with a mass ratio of 9:1 was introduced at the inlet with a velocity of 1 m/s with turbulence intensity of 20% and x-direction artificial disturbance of 0.1% of magnitude of bulk velocity. The secondary high argon concentration flow (7:3 mass ratio) was injected at the porous wall into the loop with a radial velocity of 0.002854 m/s. The Reynolds numbers at the inlet is
410 about 2,400. Note that Reynolds number is based on the inlet at large pipe.

Flow behavior and component mixing is investigated in the both "expansion-flow region" and "Dean-flow region" numerically. Figure 6 shows contour graph

of the instantaneous velocity, averaged velocity, average mass fraction of argon, and turbulence kinetic energy (TKE), respectively, in an axial planar view of the “expansion-flow region”, dashed box of inset of Figure 6. On the porous wall of location (1), highly concentrated argon gas introduced through the porous wall formed a high-concentration layer on the rim of the cross section of the pipe. Upstream of the enlarger coupling, at location (2), the concentration gradually decreases and along the wall in the flow direction. Argon was diffused radially, but it is not significant enough to mix them fully. Two different concentration layers were maintained up to the “Dean-flow-region” in the elbow. Downstream of the enlarger coupling, at location (3), the flow has two distinct concentric layers and high TKE is observed between the interfaces of the two layers due to recirculation near the corner. The reattachment point is observed at the 0.2877 m downstream of the end of the gradual expansion. Near the reattachment point, at location (4), the stratified two-layer flow becomes unstable. The flow strongly fluctuates and oscillates, referred to as localized turbulence, and thus highest TKE is observed in this region, an order of magnitude higher than that in other regions of the test facility. It may be noted that the TKE in the Figure 6-(d) is represented in log-scale. Due to turbulent mixing, it can said that the major part of component mixing is also completed in this region. However, flow distribution is little different compared with component mixing. A pair of secondary vortices, called Dean flow, are generated in the curved region (location 5), making slanted distribution of velocity profile.

Figure 7 shows contour graphs of temporally-averaged velocity and turbulence kinetic energy in the Dean-flow region. The U-shaped contour shows the axial planar view of the “Dean-flow region” and the circular contour graphs labeled as (a) to (j) show cross-sectional views at the corresponding location (A) to (J) in Figure 7. Each location is 0.1524 m apart through straight pipe and 45° apart in 90° pipe bend region. The top of the circular contour graph is facing toward the inner corner of the loop, and the black arrows in the cross-sectional views represent the direction and magnitude of the secondary flow. A pair of deformed secondary vortices are clearly observed at locations (C) and

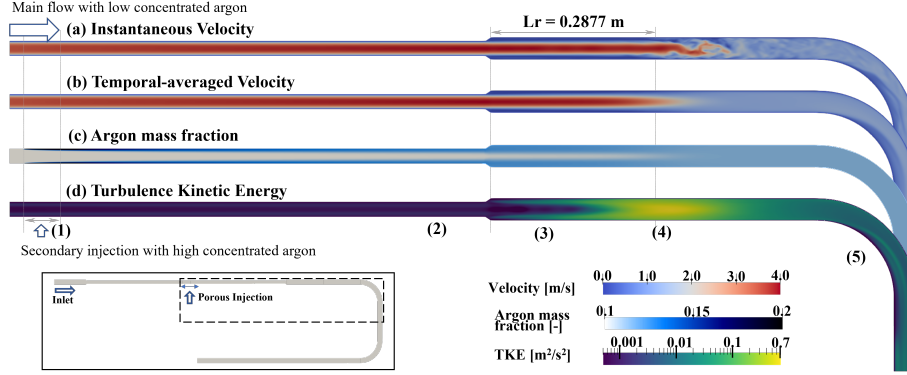


Figure 6: Contour graph for two-species simulation (a) instantaneous velocity magnitude, (b) averaged velocity magnitude, (c) averaged argon fraction, and (d) turbulence kinetic energy

(G) in Figure 7. The secondary flow at the vertical center of the cross-section moves toward the outer wall, resulting in a biased stream-wise flow at outer region of the cross-section. Flow separation and reattachment is not observed in "Dean-flow region" as Rütten et al. (2005) mentioned that no separation exists for the geometries with CR of 3.0, but there still exists a calm inner region of the cross-section and highest TKE is observed at the interface of calm region. It seems that it is related to swirl switching.

A series of elbows induces interesting flow behavior downstream of the elbow. The flow downstream of the first elbow (location E, F) is not recovered to the flow profile at location B, and as the flow approaches the second elbow, the axial velocity downstream of the second elbow (location I, J) is higher than that downstream of the first elbow. Biased main flow toward outer region of the cross-section requires a longer distance to be recovered to a fully developed flow. It can be concluded that the location at the elbow and downstream of the elbow are not good locations for measuring the velocity, temperature, or concentration.

To quantify the amount of mixing between air and argon through the loop, the AMI was introduced, defined as the Eq.5. It is the ratio of the standard deviation of the mass fraction of argon over a cross section to the averaged

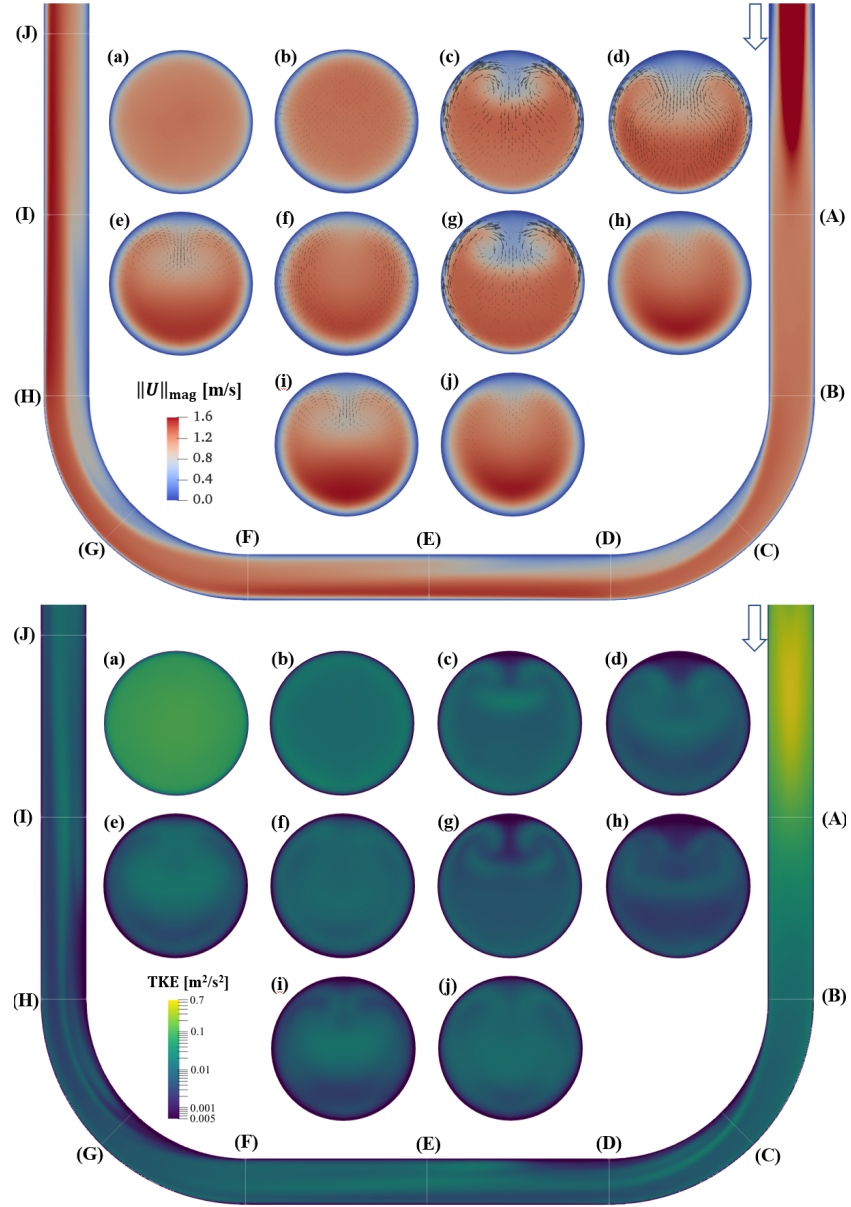


Figure 7: Contour graph of temporally-averaged velocity magnitude (top) and turbulent kinetic energy (bottom), respectively in the Dean-flow region

mass fraction over the cross section. An AMI of 0 indicates that the mixture is homogeneously mixed, while an AMI of 1 is achieved when the same amount of two materials are totally unmixed.

$$\text{AMI} = \frac{\sigma}{\langle \bar{w}_i(x, y, z) \rangle} = \frac{\sqrt{\frac{1}{A} \int_A \{\bar{w}_i(x, y, z) - \langle \bar{w}_i(x, y, z) \rangle\}^2 dA}}{\langle \bar{w}_i(x, y, z) \rangle} \quad (5)$$

where $\bar{w}_i(x, y, z)$ is the temporally averaged mass fraction of surrogate gas i at a specific point on the cross section, $\langle \bar{w}_i(x, y, z) \rangle$ is the averaged mass fraction of surrogate gas i over the cross section, σ is the standard deviation of $\bar{w}_i(x, y, z)$ over the the cross section, and A is the cross-sectional area. The value of AMI is monotonically decreasing downstream of the point of injection of the secondary flow. The slope of the AMI in the Figure 8 can be interpreted as the mixing rate. The steeper the slope is, the more rapid the mixing is.

Figure 8 represents the AMI based on the argon mass fraction along the flow loop for a given operating condition with a Reynolds number of 2,400 and with the injection of secondary gas, and slope of AMI. Red, blue, yellow and green lines of the graph represent upstream of the expansion, downstream of the expansion, first elbow, and downstream of first elbow, respectively.

At the beginning, a high concentration of argon injected through the porous wall diffuses and mixes along the flow loop. The value of AMI reaches 0.425 and starts to decrease. The mass fraction distribution has a rim with high concentration of argon, which is not mixed well. Steep slope of AMI value is observed in the location (a) of Figure 8. It looks that advection by radial velocity of the injected surrogating gas at the porous wall is the dominant reason for steep mixing in location (a) of Figure 8. As fluid flows, the effect of radial advection is attenuated and slope of AMI becomes less steep because only naturally generated turbulence eddy near the wall and molecular diffusion is dominant effects of the mixing upstream of the expansion in location (b). During gradual expansion in location (c), the distribution of the argon mass fraction is stretched out and smoothed as the diameter of the pipe increases. It is the reason that steep drop in AMI is observed at the expansion. The slope of AMI downstream of the expansion is as small as that of AMI slope in the upstream of the expansion.

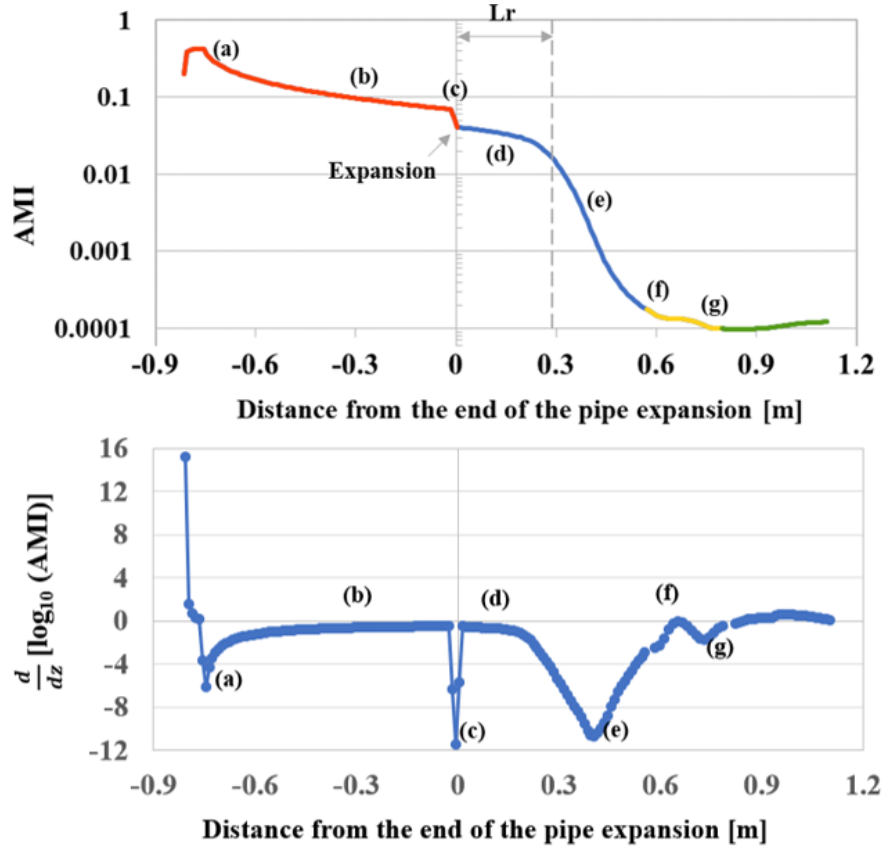


Figure 8: AMI based on argon mass fraction along the location of the loop (top) and slope of AMI (bottom)

It seems that the recirculation itself does not affect the mixing in location (d). It is supported by the result that the flow looks stratified as recirculation and mainstream flow as depicted in Figure 6-(b). The maximum change in AMI within the loop is located downstream of the expansion near the reattachment point where the localized turbulence occurs at location (e) where the turbulence intensity is order of magnitude higher than that at any other location in the LPLT FPVS. Steepest slope of AMI is located 0.40 m downstream of the expansion in location (e). Three standard deviation of the mean covers the 99.73% of normal distribution, and thus it is sufficient to state that the flow is well mixed

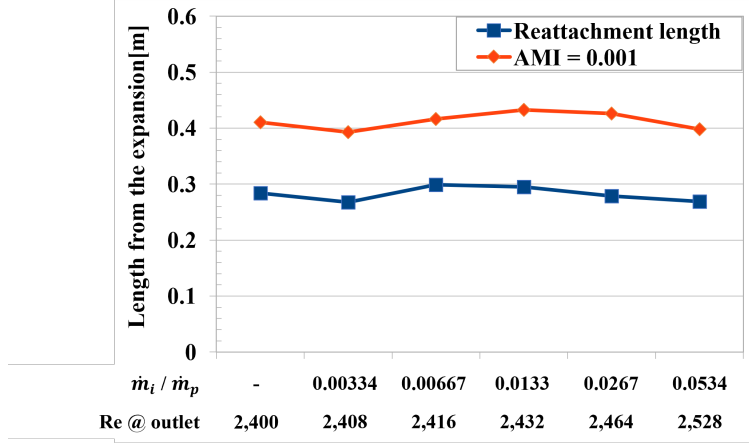


Figure 9: Reattachment and mixing lengths with different flowrate at the porous wall. $\dot{m}_i$ and $\dot{m}_p$ are flowrate at the inlet and the porous wall, respectively.

when the AMI of the argon mass fraction is below 0.001. Mixing length is defined as the length between the end of the gradual expansion and the location where AMI is 0.001 in current study. As mixing length lies between location (d) and (e), we can conclude that mixing is completed within the "expansion-flow region" upstream of "Dean-flow region". The 90 degree elbow in the "Dean-flow region" (location (g)) also have high slope of the AMI than that of the diffusion dominant regions like location (b) and (d) but it's magnitude of change is less than the change in "expansion-flow region". Rather, the redistribution of the component concentration is of interest within the elbow due to secondary flow. However, standard deviation (or AMI) cannot quantify this phenomena. The skewness of the component concentration might be required to quantify the redistribution but it is out of scope of the current study.

To check the effect of secondary injection at the porous wall on the mixing process, a sensitivity study was performed for scaled FPVS test facility. The velocity at the inlet was set at 1 m/s and a different secondary flowrate was applied at the porous wall. Figure 9 shows reattachment length (blue square) and mixing length with AMI of 0.001 (orange diamond) as a function of the flowrate ratio, defined as flowrate at the inlet over that at the porous wall.

The trend of the mixing length determined by AMI is similar to the that of
520 the reattachment length, meaning that flow behavior dominates the mixing
of components in this system. Small introduction of the flow at the porous
wall affects about 5~6% on reattachment and mixing lengths. Interestingly,
the introduction of secondary injection at the porous wall with 0.33% of bulk
mass flowrate ($\dot{m}_i$) can reduce reattachment length by 5.9% compared with no
525 injection at the porous wall introduction. In contrast, the introduction of 0.66%
bulk mass flowrate at the porous wall can increase the reattachment length by
11.7% compared with 0.33% of bulk mass flowrate at the porous wall. It seems
that the change of reattachment length by small secondary injection at the
porous wall is related to distortion of velocity profiles and increase of turbulence
530 disturbance due to the introduction of the secondary flow at the porous wall.
Further study is necessary for future studies. The decreasing trends in AMI
and reattachment length noticed in Figure 9 are attributed to increase in bulk
velocity at the axial flow.

5. Conclusions

535 CFD model combined with the solver, *reactingFOAM* and LES WALE model
in OpenFOAM v8 is validated to simulate fluid flow through a geometry of
gradual expansion pipe by comparing with (1) the PIV measurements made
by the authors and (2) other experimental and CFD results reported in litera-
ture. Axial velocity profile downstream of the expansion measured by the PIV
540 is in reasonable agreement with the LES calculations with appropriate flow dis-
turbance (turbulence intensity of 20% and x-direction artificial disturbance of
0.1% of magnitude of bulk velocity) at the inlet. The numerically predicted reat-
tachment length compares well with the experimental results at low Reynolds
numbers ranging from 1,000 to 5,000, as shown in Figure 5.

545 Using this validated model, numerical simulations were performed for the
LPLT FPVS test facility. We introduced the concept of standard deviation of
argon mass fraction over cross-section of the pipe (AMI) to quantify the mix-

ing of component and through out the loop. The value defined as the slope of $\log_{10}(AMI)$ is suggested to quantify the mixing rate in current study. High
550 component mixing is observed (1) downstream of the porous wall injection, (2) the gradual expansion joint, (3) downstream of the gradual expansion where localized turbulence is induced, and (4) downstream of the pipe bend. Highest change of $\log_{10}(AMI)$ occurred around the location (e) in Figure 8, near the reattachment of gradual expansion. As standard deviation of argon mass
555 fraction become smaller than 0.001, it can be considered that component concentration is fully mixed downstream of the location (e) in Figure 8.

However, not all downstream of the location (e) in Figure 8 is a good location to measure certain properties. The axisymmetric axial velocity distribution shifted and biased toward outer region of the cross-section at the 90° pipe bend,
560 and this biased distribution remains further downstream of the pipe bend. A series of the 90° elbow enhances biased distribution and elongates the recovery length required for velocity distribution to be fully developed downstream of the pipe bend. It can be a huge problem especially when closed loop is considered. At an elbow and downstream of an elbow is not a good location to measure flow
565 fields or mixing.

Therefore, best location to measure velocity and concentration is the location between downstream of the expansion and upstream of the first elbow, or between location (A) and (B) in Figure 7. Parametric study with different secondary flow rate shows that the trend of mixing length is similar to the
570 reattachment length. Thus, Figure 5 could suggest a specific location between location (A) and (B) in Figure 7 to measure concentration and flow rate. However, it should be noted that expansion ratio considered in Figure 5 is 2.0 while that of FPVS system is 1.5.

Since both x-direction linear disturbance and turbulence intensity is introduced at the inlet, it is hard to directly compare the numerical results with
575 experimental results. Each factor needs to be separated and studied in the future. In addition, the amount of attenuation for turbulence intensity upstream of the expansion need to be considered for better comparison in future studies.

In conclusion, the contributions of this study are: (1) validation of LES
580 to predict reattachment length downstream of the expansion by introducing
turbulence disturbance at the inlet; (2) introduction of the Absolute Mixing
Index (AMI) and it's slope to quantify component mixing and the rate of mixing,
respectively; (3) demonstration of relationship between the mixing length and
the reattachment length downstream of the expansion; and (4) identification of
585 the best location for measuring velocity and concentration in the LPLT FPVS.

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