CEDAR: A Dimensionally Adaptive Flow Solver for Cylindrical Combustors

Ty R. Hosler
Brigham Young University

Follow this and additional works at: https://scholarsarchive.byu.edu/etd

Part of the Engineering Commons

BYU ScholarsArchive Citation
https://scholarsarchive.byu.edu/etd/9337

This Thesis is brought to you for free and open access by BYU ScholarsArchive. It has been accepted for inclusion in Theses and Dissertations by an authorized administrator of BYU ScholarsArchive. For more information, please contact ellen_amatangelo@byu.edu.
CEDAR: A Dimensionally Adaptive Flow Solver for
Cylindrical Combustors

Ty R. Hosler

A thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Master of Science

Bradley R. Adams, Chair
Dale R. Tree
Scott Thomson

Department of Mechanical Engineering
Brigham Young University

Copyright © 2021 Ty R. Hosler
All Rights Reserved
ABSTRACT

CEDAR: A Dimensionally Adaptive Flow Solver for Cylindrical Combustors

Ty R. Hosler
Department of Mechanical Engineering, BYU
Master of Science

This thesis discusses the application, evaluation, and extension of dimensionally adaptive meshing to the numerical solution of velocity and pressure fields inside cylindrical reactors. Due to the high length to diameter ratios of many cylindrical reactor vessels the flow field can become axisymmetric, allowing for simplification of the governing equations and significant reduction in computational time required for solution.

A fully 3D solver is developed from existing computational tools at BYU and validated against theoretical velocity profiles for pipe flow at various Reynolds numbers, as well as with experimental data for an axial-fired center jet with recirculating flow. Dimensionally adaptive meshing is then incorporated into the validated 3D solver. The boundary conditions and assumptions at the dimensional boundary are discussed. The flow information is passed across the boundary through spatial mass-weighted averaging. The 3D and axisymmetric computational domains are decoupled from one another so information can only be passed from the 3D domain downstream to the axisymmetric domain. The dimensional boundary placement must meet two main requirements, the flow must be one-way and axisymmetric. It is found that the flow becomes axisymmetric early on in the reactor (~0.3-0.4 m), but recirculation exists farther downstream (until ~0.61 m) and thus governs the placement of the dimensional boundary.

The resulting computational tool capable of running simulations using dimensionally adaptive meshes is called CEDAR (Computationally Efficient Dimensionally Adaptive Recirculating flow solver). Several studies are then undertaken to examine CEDAR’s ability to reproduce exit velocity profiles comparable to those produced by a fully 3D mesh, including variations in pressure, firing rate, and geometry. It is found that the flow structure inside the reactor is self-similar over a wide range of operating parameters as long as the burner jets are turbulent. This observation is supported by free and confined jet theory. These theories also provide a method for placing the dimensional boundary, which is a linear function of the confining geometry diameter only (assuming that the jet diameter is less than 1/10 the diameter of the confining geometry). All exit velocity profiles produced by CEDAR are on average within 5% of the fully 3D profiles. Timing studies reveal an average 5.16 times speedup in computational time over fully 3D computations.

Keywords: CFD, dimensionally adaptive, cylindrical combustor, RANS flow solver, adaptive meshing
I would like to give a special thanks to Dr. Bradley R. Adams for his constant support, patience, and friendship over the years. His guidance and unyielding belief in me have been largely influential not only in my development as an engineer, but also as a man of faith. I wish to also thank my parents Bret and Pam for instilling in me at a young age a strong desire to learn and to work hard. Most of all I would like to thank my wife Sydney for her support, encouragement, and love during my graduate studies. Her strength and steadiness have consistently buoyed me up in the face of the many challenges of graduate school.

“This material is based upon work supported by the U.S. Department of Energy under Award Number DE-FE0029157.” Program Manager Matthew Adams.

Disclaimer: “This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.”
TABLE OF CONTENTS

ABSTRACT ................................................................................................................................. ii
TABLE OF CONTENTS ........................................................................................................ iv
LIST OF TABLES .................................................................................................................. v
LIST OF FIGURES ................................................................................................................ vi
1  Introduction ......................................................................................................................... 2
   1.1  Navier-Stokes Equation and Turbulence Modeling ..................................................... 4
   1.2  Mesh Refinement and Adaptive Dimensionality ..................................................... 5
   1.3  Objective and Scope ................................................................................................. 7
   1.4  Approach .................................................................................................................... 7
2  Development and Validation of the 3D Flow Solver ......................................................... 10
   2.1  Code Architecture and Development ..................................................................... 10
   2.2  Code Validation ...................................................................................................... 15
3  Development of CEDAR .................................................................................................. 19
   3.1  General Considerations .......................................................................................... 19
   3.2  Algorithmic Differences at the Dimensional Boundary ....................................... 21
   3.3  Boundary Conditions at the Dimensional Boundary .............................................. 24
   3.4  Determining the Dimensional Boundary Location ................................................ 25
4  Results and Discussion ..................................................................................................... 34
   4.1  General Information ............................................................................................... 34
   4.2  Runtime Dependence on Boundary Location for a Pipe Flow .............................. 36
   4.3  Parametric Study of Pressure Variation ................................................................ 38
   4.4  Parametric Study of Firing Rate .......................................................................... 44
   4.5  Runtime Dependence on 3D Domain Symmetries ................................................ 49
5  Conclusions ....................................................................................................................... 52
References .............................................................................................................................. 55
LIST OF TABLES

Table 2-1: 3D Cartesian Differential Equation Set................................................................. 11
Table 2-2: Axisymmetric Differential Equation Set................................................................. 12
Figure 1-1: A visualization of the dimensional meshing technique used by Williams and Adams [1] for the POC reactor at BYU. Note the transition from a three-dimensional cylindrical mesh to an axisymmetric and eventually one-dimensional mesh progressing axially down the reactor. ............................................................... 6

Table 2-1: 3D Cartesian Differential Equation Set ........................................................................ 11
Table 2-2: Axisymmetric Differential Equation Set .................................................................... 12

Figure 2-3: Fully developed turbulent pipe flow predictions compared with theory. ............... 16
Figure 2-4: 3D flow solver predictions compared with LDA data from Park & Chen. ............... 17

Figure 3-1: An algorithmic flowchart for CEDAR. ..................................................................... 22
Figure 3-2: Illustration of the mapping of information across the dimensional boundary from a structured 3D Cartesian mesh to an axisymmetric cylindrical mesh. Any variable (ϕ) can be mapped by mass weighted averaging over the tangential coordinate at specified radii using a constant arc length (rd0) larger than the 3D cell diagonal to avoid replicate sampling of individual cell values. ................................................................. 23

Figure 3-3: A comparison of the axial development length for the Baseline case of the study at 20 bar and the bounding case at 5 bar. Both cases can be considered axisymmetric around x = 0.35 m. ................................................................................................................................. 27

Figure 3-4: A contour plot of axial velocity at an axial position of 0.35 m. The burner central jet core is evidenced by positive velocities, whereas recirculating flow around the periphery of the reactor is evidenced by negative velocities. ................................................................. 28

Figure 3-6: A qualitative flow field visualization for a free and confined turbulent jet without and with secondary mass flow. Note the recirculation zones that develop in the near burner region close to the jet origin. Point P represents the point where the jet boundary impinges on the wall. Xp represents the axial location at which the jet spreads to the reactor radius L. A free jet would reach radius L at a shorter axial distance compared to a confined jet due to the lack of a recirculation zone from self-entrainment. Figure(s) from Barchilon and Curtet [30] ................................................................. 32

Figure 4-1: A contour plot just downstream of the reactor inlets showcasing their locations inside the POC reactor. One half of the symmetric reactor is shown in this case. Note the primary center jet (red) and four tangentially periodic secondary inlets (yellow/green). .................. 35

Figure 4-2: A non-dimensionalized plot of computational time as a function of the position of the dimensional boundary within the computational domain. ............................................................................... 36

Figure 4-3: Predicted radial profiles of axial velocity at the exit of the pipe for several of the pipe study cases with modified dimensional boundary location. ........................................................................ 37

Figure 4-4: Contour plots of normalized axial velocity inside the POC Reactor for the Pressure Study. Note that the reactor centerline is located at R = 0.1016 m in these figures. .......... 39

Figure 4-5: A tighter scale view of the normalized axial velocity inside the POC Reactor. Note the similarity in flow structure over the range of pressures used in this study. The dashed red line indicates the observed recirculation zone length (0.61 m). The reactor centerline is located at R = 0.1016 m in these figures. ................................................................. 39

Figure 4-6: Pressure contour plots for each of the pressures examined in the pressure study. ... 40
Figure 4-7: Timing results for the Pressure Variation study comparing 3D meshes with DA meshes (DA boundary at 0.701 m). ................................................................. 42

Figure 4-8: Comparison of 3D and DA mesh axial velocity profiles at the exit of the POC reactor for pressures: (a) 20 bar, (b) 10 bar, (c) 5 bar................................................................. 44

Figure 4-9: Axial velocity contour plots for the three Firing Rate cases examined in this study. Similarity of the flow is maintained even when jet Reynolds numbers are varied............... 45

Figure 4-10: A tighter scale view of the normalized axial velocity field for the Firing Rate cases. Note again the ‘ballooning’ out of the center jet beginning at ~ 0.2 m................................. 45

Figure 4-11: Timing results of the Firing Rate study comparing 3D meshes with DA meshes (DA boundary at 0.701 m). DA meshing provides a consistent speedup over its 3D counterpart. 47

Figure 4-12: Exit axial velocity profile comparisons between fully 3D and DA meshes at various Firing Rates: (a) 1.0 (100%), (b) 0.75 (75%), and (c) 0.50 (50%). .................................................... 49

Figure 4-13: Timing results for the three cases of the Geometry Study. Here again computational time decreased quadratically with cell number........................................... 50

Figure 4-14: Exit axial velocity profiles as a function of reactor radius for three domain symmetries (full geometry, half symmetry, quarter symmetry)...................................... 51
1 INTRODUCTION

Air-fired coal combustion has played, and continues to play, a significant role in the energy portfolio of many countries around the world including the United States[1]. This is in part due to coal being widely available, easily transported, and energy dense. For these reasons it is likely that coal will continue to play a large role in the energy sector for decades to come, especially in developing countries. However, despite its advantages air-fired coal combustion has fallen out of favor in many developed countries due to the amount of CO₂ emissions that it produces[2]. Ongoing research into methods to reduce the CO₂ emissions of coal has led to Pressurized Oxy-coal Combustion (POC), a promising candidate for low CO₂ emission power generation[3][4].

POC is distinct from air-fired coal combustion in several ways. First, combustors are generally cylindrical to more easily withstand the elevated operating pressures of 15-20 atms required to offset the economic costs and inefficiencies of oxygen firing. The high pressures are used to recover cycle efficiency via latent heat recovery from combustion products[5][6]. Second, to achieve gas velocities of sufficient magnitude to allow appropriate mixing/reaction, annular burner inlets have to be eliminated in favor of discrete tangentially periodic secondary inlets. Introduction of gases in this way means that the near burner region is no longer axisymmetric like in the air-fired cylindrical reactor. Third, as implied by its name POC no longer utilizes air as the oxidant in the combustion reaction, instead pure O₂ is used (in practice a
mixture of $O_2$ and $CO_2$ is used for oxidation and to control flame temperature). This reduces the number of species in the exhaust stream, which aides in simplifying $CO_2$ capture and sequestration as well as decreasing $NO_x$ emissions. One important trade off of this change in oxidant gas is that flame temperatures for POC are significantly higher than that of air-fired combustion. Therefore, flue gas recirculation in the form of $CO_2$ is commonly used to reduce temperatures inside the reactor. These characteristics of POC mean that the physics of the problem (i.e. fluid flow, reactions, radiation, particle transport, etc.) differ significantly from those of air-fired combustion. Gaining greater insight into these phenomena in the context of POC is essential to its successful implementation around the world.

The tremendous advances in memory and speed of computers in recent history has made them increasingly accessible as advanced engineering tools. These improvements coupled with the decreasing capital cost of computers has led to their becoming a more commonplace tool in modeling industrial processes. Coal combustion is one such application. Coal combustion includes a wide array of physics (fluid flow, heat transfer, mass transfer, chemical kinetics, etc.) and thus its computational treatment can be quite complex. Comprehensive models often include several sub-models with each addressing a different facet of the flow. While these comprehensive CFD (Computational Fluid Dynamics) models can vary widely in their approach, they all generally require a substantial amount of computational resource and time. However, this cost is not set. Informed modeling decisions and methods can significantly decrease it. To successfully accomplish this requires careful observation and judgement on the part of the modeler. Williams and Adams [7] have successfully demonstrated this concept by using a Dimensionally Adaptive (DA) meshing technique to significantly reduce the computational resources required for solution of the radiation field in a cylindrical pressurized oxy-coal reactor.
The major objective of this work has been implementing and extending this DA meshing technique to the solution of the flow field inside a cylindrical pressurized reactor for non-reacting flow.

1.1 Navier-Stokes Equation and Turbulence Modeling

The governing equation of motion for any fluid is the Navier-Stokes equation, which has the following general form for an incompressible fluid:

\[
\rho \left( \frac{\partial u_i}{\partial t} + U_j \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_i^2} + \rho g_i
\]  

(1-1)

This equation is valid for all incompressible flows, including turbulent ones. However, the number of computational cells and time steps required to adequately resolve the scales inherent in turbulent flows in industrial systems is beyond the current capabilities of even the largest supercomputers. However, for most engineering flows average values of various parameters prove sufficient. Averaging the Navier-Stokes equations results in the Reynolds averaged Navier-Stokes (RANS) equation:

\[
\rho \left( \frac{\partial \bar{u}_i}{\partial t} + \bar{U}_j \frac{\partial \bar{u}_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 \bar{u}_i}{\partial x_i^2} - \frac{\partial (\rho \bar{u}_i \bar{u}_j)}{\partial x_j} + \rho g_i
\]  

(1-2)

The Reynolds averaged Navier-Stokes equation allows computation of the average quantities for the flow of interest, provided a turbulence closure method is used for approximation of the new Reynolds stress term now present on the right hand side (RHS).

The flow field in the reactor determines the distribution of coal particles and the mixing of fuel and oxidizer. This in turn determines the flame location and therefore the temperature and radiation profiles inside the reactor. Accurate characterization of the flow field is therefore an
essential step in properly describing the coupled physics of reactors. Modeling of turbulent flows requires balancing model accuracy and computational efficiency. These trade-offs occur during the selection of turbulence models and computational mesh refinements. Numerous models have been constructed in an attempt to resolve turbulence effects, from zero equation models up to the popular k-ε two equation model [8] and beyond. Each model has various strengths and weaknesses. Higher fidelity models offer better resolution at a higher computational cost, while lower order models offer decreased cost, but at lower resolution[9][6][10]. Gillis and Smith noted that the turbulence sub-model was the limiting factor for convergence in their flow modeling investigations[11]. Recent literature has shown that turbulence modeling in industrial applications is still largely RANS based, with preference for the two equation k-ε model and its variations [12][9]. This suggests that higher order models and methods, while providing greater detail and insight, incur too high a cost (whether computational memory or time) to be viable for industrial applications as was needed for this work. Therefore, the k-ε model was used in this work because it has the capability of resolving recirculation zones and turbulent mixing at reasonable computational cost.

1.2 Mesh Refinement and Adaptive Dimensionality

Adaptive Mesh Refinement (AMR) is a popular method in Computational Fluid Dynamics (CFD) modeling in which the mesh is locally refined to resolve high gradients within the computational domain. This allows a judicious placement of nodes to sufficiently resolve flow gradients while minimizing the overall number of computational points. While there are many mesh refinement techniques, two general approaches exist within this field[13]. In the first approach additional nodes are added to high gradient regions in the flow, or in other words the
mesh is locally refined[14]. The second approach repositions a constant number of computational points within the domain to better resolve gradients, but results in a “coarsening” of the mesh elsewhere. Recently, Williams and Adams [7] proposed the use of a novel Dimensionally Adaptive (DA) mesh for the rapid solution of radiative heat transfer in a cylindrical geometry (illustrated in Figure 1-1). They observed that the large length to diameter ratios of most cylindrical pressurized reactors allows for the flow to develop to the point that it eventually becomes axisymmetric and even one-dimensional near the end of the reactor (see Figure 1-1). With this observation, they then constructed a DA mesh to explore the possible time and computational savings associated with radiative heat transfer calculations. This work seeks to apply this meshing technique to the solution of the flow (i.e. provide resolution of velocity and pressure fields) and extend it through the development of a physics based algorithm to determine dimensional mesh boundaries a priori.

Figure 1-1: A visualization of the dimensional meshing technique used by Williams and Adams [1] for the POC reactor at BYU. Note the transition from a three-dimensional cylindrical mesh to an axisymmetric and eventually one-dimensional mesh progressing axially down the reactor.
1.3 Objective and Scope

The main objective of this research program is the application, extension, and assessment of a Dimensionally Adaptive (DA) [7] meshing technique (illustrated in Figure 1-1) to help speed the solution of non-reacting pressurized fluid flow in a cylindrical combustor geometry with non-axisymmetric inlet flows.

The application was the development of a RANS solver for the POC reactor at BYU (a cylindrical geometry with top inlets and a bottom outlet). The extension was the application of DA meshing to flow equations as well as the development of a physics-based algorithm to determine dimensional mesh boundaries \textit{a priori}. The assessment included evaluation of the accuracy and computational efficiency of a turbulent flow solver for a DA mesh in a cylindrical geometry (3D to axisymmetric flow was explored, consideration and calculation of flow field transition to 1D from axisymmetric was not done in order to maintain the predictive capability of radial variation until the exit of the reactor). It should be noted that while this flow solver could eventually become part of a larger multi-physics CFD code, no particle flow or chemical reactions were considered as part of this work. Additionally, the dimensional boundary locator was developed using non-reacting flow correlations.

1.4 Approach

Pursuant to the main research objective of this research program, several research tasks were set: (1) develop or obtain source code for a 3D turbulent flow solver, (2) validate the 3D turbulent flow solver using published jet profile data, (3) modify the validated flow solver to accommodate DA meshes, (4) compare DA calculation accuracy and computational time with
the validated fully 3D results, (5) develop a dimensional boundary locator algorithm based on non-reacting jet theory correlations.

The first research task consisted of examining several turbulent flow solvers that could serve as the base for which DA meshing capabilities (see Figure 1-1) could be added. In general, the solver needed to be capable of accurately resolving confined turbulent recirculating flows in cylindrical geometries. In addition to this, it also needed to possess the functionality to handle flow-field obstructions, multiple inlets, and symmetry boundary conditions. Two previously developed BYU CFD codes (gas3D and PCGC-3) contained all the necessary software architecture for a 3D RANS flow solver with these capabilities and thus served as the basis for the development of the Computationally Efficient Dimensionally Adaptive Recirculating (CEDAR) flow solver. More details about CEDAR will be discussed in the third section (3 Development of CEDAR) of the thesis.

Whenever a new computational tool is developed it must be validated so that modelers can be confident that the results obtained from the model approach those of the physical system it is representing. In the case of CEDAR, this physical system of interest includes recirculating confined flows produced by jets issuing into a sudden expansion. Thus, comparison of the predictions of CEDAR with published confined jet flow data was performed to assure that the tool was providing physically realistic results and trends.

After validation of fully 3D and axisymmetric predictions, CEDAR was further developed to accommodate DA meshing. Preliminary assessment of simple DA cases (pipe flow and a centrally located jet issuing into a sudden expansion) were undertaken and the results are presented in Section 3 of the thesis along with details about the development and integration of dimensional adaptivity into the solver.
A series of studies were then undertaken for the more complex case of the POC reactor geometry. Pressure, geometry, and firing rate studies were all undertaken to allow for comparison and assessment of the timing and accuracy differences of DA cases with fully 3D results. Lastly, analysis of the data from the various studies along with classical jet theory was used to extend dimensional meshing by developing an algorithm for the \textit{a priori} placement of the dimensional boundary.
2 DEVELOPMENT AND VALIDATION OF THE 3D FLOW SOLVER

This section of the thesis discusses the development, architecture and capabilities, and validation of the 3D flow solver developed for this work.

2.1 Code Architecture and Development

The 3D flow solver developed shares most of its internal architecture with two CFD codes previously developed at BYU (PCGC-3 and gas3D). It discretizes the governing Navier-Stokes momentum PDEs on a staggered structured polyhedral grid using the SIMPLER algorithm [15][16]. Upwind/central differencing are used for the calculation of convection and diffusion coefficients. All the governing PDEs can be set into the same general equation form shown on the top line of Table 2-1 and Table 2-2. Setting the equations in this form allows for a single matrix solver to be utilized for their solution. The discretized set of linear equations is solved using a Tri-Diagonal Matrix Algorithm (TDMA) [17]. Early CFD investigations by Reaction Engineering International (REI) of a POC design concept (see Figure 2-1) suggested that recirculation zones would be present in the reactor, thus requiring a turbulence model to be capable of resolving such flows. As previously stated, turbulence closure is achieved through the linear k-ε model with the recommended standard constant values. Near boundaries a wall function is employed to avoid the computational cost of integrating the boundary layer equations to resolve the gradients near the wall.
Table 2-1: 3D Cartesian Differential Equation Set

\[
\frac{\partial(\rho \bar{u} \phi)}{\partial x} + \frac{\partial(\rho \bar{v} \phi)}{\partial y} + \frac{\partial(\rho \bar{w} \phi)}{\partial z} - \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial y} \left( \Gamma \frac{\partial \phi}{\partial y} \right) - \frac{\partial}{\partial z} \left( \Gamma \frac{\partial \phi}{\partial z} \right) = S_\phi
\]

<table>
<thead>
<tr>
<th>Equation</th>
<th>( \phi )</th>
<th>( \Gamma_\phi )</th>
<th>( S_\phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>X Momentum</td>
<td>( \bar{u} )</td>
<td>( \mu_e )</td>
<td>(- \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( \mu_e \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_e \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_e \frac{\partial \bar{u}}{\partial z} \right) + r \bar{\rho} g_x - \frac{2}{3} \bar{\rho} \tilde{k} )</td>
</tr>
<tr>
<td>Y Momentum</td>
<td>( \bar{v} )</td>
<td>( \mu_e )</td>
<td>(- \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \mu_e \frac{\partial \bar{v}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_e \frac{\partial \bar{v}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_e \frac{\partial \bar{v}}{\partial z} \right) + r \bar{\rho} g_y - \frac{2}{3} \bar{\rho} \tilde{k} )</td>
</tr>
<tr>
<td>Z Momentum</td>
<td>( \bar{w} )</td>
<td>( \mu_e )</td>
<td>(- \frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left( \mu_e \frac{\partial \bar{w}}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_e \frac{\partial \bar{w}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_e \frac{\partial \bar{w}}{\partial z} \right) + r \bar{\rho} g_z - \frac{2}{3} \bar{\rho} \tilde{k} )</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>( \bar{\tilde{f}} )</td>
<td>( \frac{\mu_e}{\sigma_f} )</td>
<td>0</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>( \bar{\tilde{g}} )</td>
<td>( \frac{\mu_e}{\sigma_g} )</td>
<td>( c_{g1} \mu_e \left[ \left( \frac{\partial \bar{\tilde{f}}}{\partial x} \right)^2 + \left( \frac{\partial \bar{\tilde{f}}}{\partial y} \right)^2 + \left( \frac{\partial \bar{\tilde{f}}}{\partial z} \right)^2 \right] - c_{g2} \bar{\rho} \bar{\tilde{g}} \frac{\bar{\tilde{e}}}{\bar{k}} )</td>
</tr>
<tr>
<td>Variance</td>
<td>( \bar{\tilde{k}} )</td>
<td>( \frac{\mu_e}{\sigma_k} )</td>
<td>( (G - \bar{\rho} \bar{\tilde{e}}) )</td>
</tr>
<tr>
<td>Turbulent Energy</td>
<td>( \bar{\tilde{\varepsilon}} )</td>
<td>( \frac{\mu_e}{\sigma_\varepsilon} )</td>
<td>( \left( \frac{\bar{\tilde{e}}}{\bar{k}} \right) (c_1 G - c_2 \bar{\rho} \bar{\tilde{e}}) )</td>
</tr>
</tbody>
</table>

Where:

\[
g = \mu_e \left\{ 2 \left[ \left( \frac{\partial \bar{u}}{\partial x} \right)^2 + \left( \frac{\partial \bar{v}}{\partial y} \right)^2 + \left( \frac{\partial \bar{w}}{\partial z} \right)^2 \right] + \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right)^2 + \left( \frac{\partial \bar{u}}{\partial z} + \frac{\partial \bar{v}}{\partial x} \right)^2 + \left( \frac{\partial \bar{v}}{\partial z} + \frac{\partial \bar{w}}{\partial y} \right)^2 \right\}
\]
**Table 2-2 : Axisymmetric Differential Equation Set**

\[
r \frac{\partial (\rho \tilde{u} \phi)}{\partial x} + \frac{\partial (\rho r \tilde{v} \phi)}{\partial r} - r \frac{\partial}{\partial x} \left( \Gamma_\phi \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left( r \Gamma_\phi \frac{\partial \phi}{\partial r} \right) = S_\phi
\]

<table>
<thead>
<tr>
<th>Equation</th>
<th>( \phi )</th>
<th>( \Gamma_\phi )</th>
<th>( S_\phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>X Momentum</td>
<td>( \tilde{u} )</td>
<td>( \mu_e )</td>
<td>(-r \frac{\partial p}{\partial x} + r \frac{\partial}{\partial x} \left( \mu_e \frac{\partial \tilde{u}}{\partial x} \right) + \frac{\partial}{\partial r} \left( \mu_e r \frac{\partial \tilde{v}}{\partial x} \right) + r \rho g_x - \frac{2}{3} r \rho k)</td>
</tr>
<tr>
<td>R Momentum</td>
<td>( \tilde{v} )</td>
<td>( \mu_e )</td>
<td>(-r \frac{\partial p}{\partial r} + r \frac{\partial}{\partial x} \left( \mu_e \frac{\partial \tilde{u}}{\partial r} \right) + \frac{\partial}{\partial r} \left( \mu_e r \frac{\partial \tilde{v}}{\partial r} \right) - \frac{2}{3} \mu_e \rho \tilde{v} + \rho g_r - \frac{2}{3} r \rho k)</td>
</tr>
<tr>
<td>( \theta ) Momentum</td>
<td>( \tilde{w} )</td>
<td>( \mu_e )</td>
<td>(-\rho \tilde{w} - \frac{\partial}{\partial r} \left( \mu_e \right) + \rho g_\theta - \frac{2}{3} r \rho k)</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>( \tilde{f} )</td>
<td>( \frac{\mu_e}{\sigma_f} )</td>
<td>0</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>( \tilde{g} )</td>
<td>( \frac{\mu_e}{\sigma_g} )</td>
<td>( c_g \mu_e r \left( \frac{\partial \tilde{f}}{\partial x} \right)^2 + \left( \frac{\partial \tilde{f}}{\partial r} \right)^2 ) - ( c_g \frac{2}{3} r \rho \tilde{g} \frac{\tilde{e}}{k} )</td>
</tr>
<tr>
<td>Variance</td>
<td>( \tilde{k} )</td>
<td>( \frac{\mu_e}{\sigma_k} )</td>
<td>( r (G - \rho \tilde{e}) )</td>
</tr>
<tr>
<td>Turbulent Energy</td>
<td>( \tilde{\epsilon} )</td>
<td>( \frac{\mu_e}{\sigma_\epsilon} )</td>
<td>( \left( \frac{\tilde{\epsilon}}{k} \right) (c_1 G - c_2 \rho \tilde{\epsilon}) )</td>
</tr>
<tr>
<td>Dissipation Rate</td>
<td>( \tilde{\epsilon} )</td>
<td>( \frac{\mu_e}{\sigma_\epsilon} )</td>
<td>( \left( \frac{\tilde{\epsilon}}{k} \right) (c_1 G - c_2 \rho \tilde{\epsilon}) )</td>
</tr>
</tbody>
</table>

Where:

\[
G = \mu_e \left\{ 2 \left[ \left( \frac{\partial \tilde{u}}{\partial x} \right)^2 + \left( \frac{\partial \tilde{v}}{\partial r} \right)^2 + \left( \frac{\partial \tilde{w}}{\partial x} \right)^2 + \left( \frac{\partial \tilde{v}}{\partial x} + \frac{\partial \tilde{u}}{\partial r} \right)^2 + \left( \frac{\partial \tilde{w}}{\partial x} + \frac{\partial \tilde{v}}{\partial r} \right)^2 + \left( \frac{\partial \tilde{w}}{\partial x} \right)^2 \right] \right\}
\]
Figure 2-1: CFD results of an early cylindrical reactor design showing axial velocity. In the left figure, blue regions indicate upward velocity (recirculation) whereas red regions indicate downward velocity. The top right figure shows surface contours of axial velocity for the central and secondary jets illustrating the three dimensionality of the flow in the near burner region. The bottom right figure shows a representation of the DA mesh used to simulate the reactor geometry. CFD simulation conducted by REI.

In addition to the solution of the native variables (pressure and velocities), turbulence and gas mixture variable fields are also resolved (turbulent kinetic energy, $k$, turbulent eddy dissipation, $\varepsilon$, gas mixture fraction, $f$, gas mixture fraction variance, $g$). Transport equations for $f$ and $g$ were included in anticipation of this tool possibly becoming part of a larger CFD code. Thus, the 3D flow solver also has the capability to handle variable density flows. Flow-field obstructions, multiple inlets/streams, and symmetry boundary conditions are also supported.
As the 3D flow solver may become part of a larger combustion model, it needed to be developed with this goal in mind. PCGC-3 and gas3D are written in the FORTRAN coding language, but the 3D flow solver was developed using the open-source PYTHON coding language to allow it to more easily interface with the already developed radiative heat transfer sub-model. This required porting significant portions of gas3D and PCGC-3 from FORTRAN into PYTHON. Upon completion of the porting process however it was observed that the PYTHON code execution time was significantly slower than equivalent FORTRAN scripts.

There are a variety of reasons attributed to this poor numerical performance, the most prominent of which is the fact that PYTHON is an interpreted language. This means that PYTHON code is not compiled on machine like FORTRAN but is read and executed by another program known as the “interpter”. This results, generally, in PYTHON being an excellent language for rapid prototyping and development of scripts, but a poor performer when it comes to numerical calculation. Thankfully, due to PYTHON’s widespread use among the scientific community this issue has received a lot of attention. Several options currently exist that seek to address this issue directly. The option employed in the 3D flow solver is called NUMBA [18]. The NUMBA JIT (Just in Time) compiler converts a subset of PYTHON numpy code to optimized machine language at runtime using the LLVM compiler library. Implementation of the NUMBA JIT compiler resulted in a 200-300% speedup in the 3D flow solver runtimes, bringing its computation speed back on par with compiled languages designed for numerical calculation such as C++ and FORTRAN.
2.2 Code Validation

After the successful implementation of the NUMBA JIT compiler, validation of the 3D flow solver was able to proceed. Figure 2-2 and Figure 2-3 show similarity profiles of axial velocity for fully developed pipe flow at two different Reynolds numbers, one laminar and one turbulent compared with theoretically predicted profiles. In both cases the calculated velocity profile is in good agreement with those predicted by theory [19].

The turbulent flow predictions are seen to slightly overestimate velocities near the centerline but are still in good agreement with theory. These cases illustrate the 3D flow solver's ability to reproduce developed flow profiles correctly and accurately over a wide range of conditions.

![Velocity Predictions](image)

**Figure 2-2:** Fully developed laminar pipe flow predictions compared with theory.
Next, the 3D flow solver’s ability to resolve turbulent recirculating flows was examined. Park & Chen [20] measured and simulated turbulent recirculating flow for a centrally located annulus issuing into a sudden expansion. Two different flows were studied in the paper, one where the entrance velocities of the annulus and jet were the same, and one in which they were not. The case in which the entrance velocities were the same was reproduced in this work.

Figure 2-4 shows the comparison between the 3D flow solver axial velocity predictions and the laser Doppler anemometry (LDA) measurements produced by Park & Chen. Note that negative $U/U_c$ values indicate reverse flow in Figure 2-4. Generally, the results are in good agreement with the measurements except around the recirculation zone attachment point (see x/d profiles 11.22 and 14.37). These profiles show that the 3D flow solver under predicts the recirculation zone length. This under prediction of the recirculation zone length is expected as it was also observed by Park & Chen in their numerical investigations of the same flow.
Figure 2-4: 3D flow solver predictions compared with LDA data from Park & Chen.
Besides the expected under prediction of the recirculation zone length, the good agreement of the 3D flow solver with experimental data is quite encouraging. Recirculation in the near burner region is correctly reproduced, as well as the spreading behavior of the jet (as evidenced by the flattening of velocity profiles as x/d increases). It should be mentioned however, that the under prediction of the recirculation zone (see x/d = 11.22 and 14.37) suggests that the spreading rate is over predicted. This conclusion is supported by the observations of others [20][21]. This is important to note because it has implications for the placement of the DA mesh boundary within the computational domain which will be discussed in Section 3 of the thesis.

Lastly, it is worth pointing out the rapid development of the axial flow profile within the reactor. Before even reaching halfway down the reactor length the radial profile of axial velocity is largely uniform and it stays this way until the exit. This suggests that axisymmetric calculations for this region of flow inside the reactor could substantially decrease computational effort without a significant loss in accuracy. This will be explored further in Section 3 of the thesis where the development and incorporation of DA meshing into the 3D flow solver is discussed and a new computational tool is created for the investigation of DA meshing in cylindrical environments.
3 DEVELOPMENT OF CEDAR

This section discusses the integration of DA meshing technique into the 3D flow solver resulting in the creation of CEDAR (Computational Efficient Dimensionally Adaptive Recirculating flow solver).

3.1 General Considerations

A DA mesh constitutes a mesh which partitions the full computational domain into subdomains according to the dimensionality of the flow. For cylindrical down fired reactors such as those encountered in POC the flow can generally be subdivided into two and possibly even three subdomains depending on the length to diameter ratios and burner design of the reactor. The fully 3D domain consists of the region of flow where three-dimensional effects are present and strongly influence the character of the flow. For POC reactors this is the near burner region. Intense mixing, recirculation, and shear flow can and does exist in this region, thus three-dimensional calculations are needed to accurately characterize the flow in this domain.

Next is the axisymmetric flow region. This region’s existence is not guaranteed for every flow, but for cylindrical reactors with $L/D \geq 5.85$ (as is the case for this research) its development is a physical certainty. This region of flow is characterized by an absence (or near absence) of tangential variation in the flow. Mathematically this is represented by Equation 3-1 below.
\[
\frac{1}{r} \frac{\partial \phi}{\partial \theta} = 0 \tag{3-1}
\]

where \( \phi \) is the sensitivity variable in determining the periodicity of the flow (for this work the axial velocity \( U \) served as \( \phi \)). Due to the zero (or near zero) value of this term, its contribution in the equations listed in Table 2-1 can safely be neglected. This greatly simplifies the equations and the accompanying calculations (see Table 2-2). Two less coefficients are now calculated at each computational node and one less directional sweep for each solver iteration of each variable must be performed, further aiding in a decrease in the total computational resource required.

Last is the one-dimensional or plug flow domain. While investigation of this phenomena is beyond the scope of this work, theoretically if the reactor is long enough the flow can develop to the point that it no longer varies tangentially or radially as shown in Equation 3-2.

\[
\frac{1}{r} \frac{\partial \phi}{\partial \theta} = \frac{1}{r} \frac{\partial \phi}{\partial r} = 0 \tag{3-2}
\]

At this point only variation in the axial direction of the flow must be accounted for. As a result, even further reduction in the computational complexity of the problem is possible for sufficient resolution of the flow field in this region. In a cylindrical reactor these calculations would be carried out until the exit of the reactor itself. For this work it was desired that the possibility of predicting radial profiles at the exit of the reactor be preserved, and thus 1D flow was not considered as part of this work.

The preceding discussion highlights the general philosophy of a DA mesh and is simple to understand. However, in practice this ideology requires consideration of several important factors: Where and how to place dimensional boundaries? What boundary conditions exist at dimensional boundaries? How is information mapped across dimensional boundaries? How do calculation routines change as dimensional boundaries are crossed? The remainder of this section
is dedicated to showing how these questions were handled and ultimately how DA meshing was incorporated into the 3D flow solver resulting in the new computational tool CEDAR.

3.2 Algorithmic Differences at the Dimensional Boundary

For DA meshed cases in CEDAR, the computational domain is decomposed into two regions, the fully 3D region and the fully axisymmetric region. These two domains meet at the dimensional boundary, with the 3D region always being located upstream of the axisymmetric region. CEDAR currently uses one-way coupling between the two calculation domains. This means that CEDAR first resolves the fully 3D flow domain before passing on the necessary inputs for the solution of the axisymmetric domain (see Figure 3-1, Figure 3-2), and assumes that all axial flow at the outlet of the 3D domain is moving downstream. This assumption is particularly relevant when selecting the dimensional boundary. Figure 3-1 illustrates the algorithm used to calculate the flow fields in the 3D and axisymmetric domains. Figure 3-2 illustrates how variables are passed (mapped) between the 3D domain and axisymmetric domain. All variables ($\phi$) are mapped by calculating the mass flow weighted average of the variable over the tangential coordinate at specified radii at the outlet of the 3D domain. This average value is assigned as an inlet condition to the axisymmetric domain as a function of radius. Variables in the 3D domain are evaluated at the specified radii using a constant arc length ($rdO$) larger than the 3D cell diagonal to avoid replicate sampling of individual cell values. The mesh refinement of the axisymmetric domain is chosen to match the mesh refinement of the 3D domain from reactor centerline to outer surface on a one-to-one basis.
Figure 3-1: An algorithmic flowchart for CEDAR.
**Figure 3-2:** Illustration of the mapping of information across the dimensional boundary from a structured 3D Cartesian mesh to an axisymmetric cylindrical mesh. Any variable ($\phi$) can be mapped by mass weighted averaging over the tangential coordinate at specified radii using a constant arc length ($rdo$) larger than the 3D cell diagonal to avoid replicate sampling of individual cell values.

Within the fully 3D domain six neighbor coefficients plus source terms are required for the solution of a specific variable at each node point within the domain as required by the SIMPLER algorithm. Sweeps in the X, Y, and Z directions are performed by the TDMA solver in the 3D domain. All calculations within this domain are performed on a 3D structured Cartesian mesh. Conversely, within the axisymmetric domain only four neighbor coefficients plus source terms are required for a variable’s solution. Additionally, only two directional sweeps are needed within the solver (X, R). All calculations within this domain are performed in axisymmetric cylindrical coordinates.
3.3 Boundary Conditions at the Dimensional Boundary

The dimensional boundary is treated as a conventional outlet plane in the 3D domain. This means that the exit plane (i.e., Nth plane) $\phi$’s are set equal to the N-1 plane $\phi$’s (i.e., the axial variation is zero or close to it). This of course is an approximation, but becomes increasingly accurate as the mesh spacing is reduced, and/or as the flow becomes fully developed. This boundary condition is commonly used in CFD simulations because it does not require knowledge of any variables at the exit plane of the domain since they are assumed equal to those values just upstream [22][23]. However, this implies that the flow field at the dimensional boundary is parabolic (i.e. one-way). This is obviously not true if the boundary is placed within a recirculating region within the flow. This observation plays a critical role in determining the boundary location and is discussed further in the next section of the thesis.

On the axisymmetric side, the dimensional boundary acts as an inlet plane. Mass-weighted averages computed from the 3D side are set as the input values for the domain. As the calculations in this domain are performed assuming an axisymmetric flow, more accurate predictions can be expected if the dimensional boundary is placed at a point in the overall domain where the flow is indeed axisymmetric (in other words, the tangential variation of the flow is small). Like the prescribed input values for the 3D domain, once calculated, the “inlet” values for the axisymmetric domain are set and do not change. Again, it should be mentioned that because the axisymmetric calculations are only performed once the 3D domain has been converged, no information is allowed to travel back upstream from the axisymmetric domain.
3.4 Determining the Dimensional Boundary Location

In light of the discussion above the ideal location (i.e., the location that yields the maximum computational time reduction with minimal accuracy loss, determined here by the average error in the radial profile of the axial velocity at the exit of the reactor) for the dimensional boundary is at a point in which the flow is one-way and axisymmetric. One-way flow (i.e., no recirculation) ensures that the 3D and axisymmetric domain calculations can be decoupled. The mapping technique used ensures that the field variables at the exit of the 3D domain are accurately represented at the inlet of the axisymmetric domain. These requirements (one-way flow and one-one mapping) imply then that the dimensional boundary cannot be placed within a recirculation zone, or at a position in the flow with high tangential gradients. If either of these conditions exist at the dimensional boundary location, the assumptions and boundary conditions there are not guaranteed to convey information across the boundary accurately. Thus, determining the best placement of the dimensional boundary becomes equivalent to answering the following questions: At what axial position does the flow become axisymmetric inside the reactor? At what axial location does the recirculation zone due to inlet jet entrainment end? Which of the two is the limiting factor?

3.4.1 Periodicity

When does the flow in the reactor become axisymmetric? This depends on several factors such as: burner configuration, reactor geometry, fluid properties, and firing rates. However, using the standard deviation of the periodicity factor \( \left( \frac{1}{r} \frac{\partial \phi}{\partial \theta} \right) \) evaluated at each axial layer of the mesh, the axial position at which the flow becomes axisymmetric can be found. Use of the standard deviation is preferred as it provides a consistent manner in which transition to
axisymmetric flow can be predicted. This is because at any given axial plane the periodicity factor at a point can take on both positive and negative values. Therefore, simply looking at the mean value of the periodicity factor can be misleading as a zero value would appear to indicate axisymmetric flow at that location. This isn’t always true however, as the possibility of negative and positive values means that the average can become zero due to cancellation. The standard deviation avoids this issue regardless of the average as it measures the “spread” of the sample about the mean. For an ideal axisymmetric flow, the mean periodicity and standard deviation would both be zero, thus by using the standard deviation as the flow axisymmetry measure and observing the axial location at which it takes on a subjectively low value, consistent prediction of the axial location at which transition to axisymmetric flow occurs can be obtained. For the specific geometry of this work, calculation of this factor at the radius of the secondary inlets is the best choice as that is where the highest periodicity occurs. As mentioned above as the standard deviation of the periodicity factor approaches zero (for this work when $\frac{1}{r} \frac{\partial \phi}{\partial \theta} < 0.05$) this signifies a decreasing dependency of $\phi$ on $\theta$. Again, the $\phi$ of interest in this work is the axial velocity, $U$. At this point it is reasonable to assume that the flow has become axisymmetric and theoretically will incur no accuracy penalty by switching to purely axisymmetric calculations.

It can be seen in Figure 3-3 that for the bounding case in the study (i.e., the largest inlet velocities) at a pressure of 5 bar, the axial distance over which the flow becomes axisymmetric is virtually identical to the most typical case of the study (i.e., the same geometry and flow rates at 20 bar). This indicates that the entrance length for the flow to become axisymmetric (for this burner configuration) is much more sensitive to geometry than flow conditions. It should also be noted that the development length for the flow to become functionally axisymmetric is quite small (~0.3-0.4 m, 20-25% of the reactor length). This observation validates the use of a DA
mesh to speed solution time. As axisymmetric development length is observed to be a stronger function of geometry than flow parameters, one would expect the burner design to have a strong influence on the axisymmetric flow development. Intuitively then, as burner design itself becomes more axisymmetric (i.e., moving from discrete tangential lances towards a continuous annulus) the axisymmetric development length is expected to trend towards zero. Conversely, development length can be expected to increase as burner design diverges away from symmetry.

![Graph](image)

**Figure 3-3**: A comparison of the axial development length for the Baseline case of the study at 20 bar and the bounding case at 5 bar. Both cases can be considered axisymmetric around $x = 0.35$ m.

In relation to the above discussion it is tempting to say that the dimensional boundary can be placed ~0.3-0.4 m from the burner inlet. However, it is important to recall the conditions and assumptions at the dimensional boundary. Specifically, in this instance it must be remembered that the dimensional boundary in CEDAR currently decouples the 3D and axisymmetric domains. As previously stated, for this approach to provide physically realistic and accurate
results the flow must also be one-way at the boundary. At the axial locations where the flow is observed/predicted to transition to axisymmetric flow, recirculation exists (see Figure 3-4 below). Therefore, placement of the dimensional boundary at these axial locations would violate this requirement.

![Figure 3-4](image)

**Figure 3-4:** A contour plot of axial velocity at an axial position of 0.35 m. The burner central jet core is evidenced by positive velocities, whereas recirculating flow around the periphery of the reactor is evidenced by negative velocities.

### 3.4.2 Recirculation zone length

When does the recirculation zone end? The existence of recirculation at the point in the flow at which it becomes axisymmetric means that the recirculation zones are the limiting factor in placing the dimensional boundary. This means that for the POC geometry, being able to reliably predict the recirculation zone length is equivalent to knowing where to place the dimensional boundary.
Classical jet theory may be used to understand and predict the recirculation zone lengths in the reactor [24][25] as the burner jets are the reason for the development of recirculation zones. In the case of a free jet, it can be shown that the total jet momentum is conserved and thus the centerline velocity decay and spreading rates are linear functions of axial distance (x) from the origin of the jet[26]. The centerline velocity decay is inversely proportional to axial distance and the spreading rate of the jet is directly proportional to it. Additionally, using the jet half angle (defined as the radial location at which axial velocity takes on half of the centerline value) it can be shown that the spreading angle of any turbulent free jet is 12.5°[27]. This result suggests that regardless of flow rate, any two jets issuing from the same size orifice will, if they are turbulent, spread at exactly the same rate. Using the above spreading angle, a relationship can be derived that gives the axial location, $X_p$, at which the jet radius reaches an arbitrary radius $L$:

$$X_p = 4.5L$$

(3-3)

If $L$ is taken to be the radius of a cylindrical reactor, the above expression then yields the axial location at which a free jet would hypothetically impinge on the walls of an enclosing reactor. However, due to the enclosing reactor walls the amount of mass available for the jet to entrain is limited and thus the jet spreading behavior is expected to change due to the presence of the reactor walls.

The effects of confinement on jet spreading behavior has been explored by Thring and Newby [28] as well as others [29][30]. Experimental measurements show that the presence of the walls narrows the jet spreading angle of turbulent confined jets to 9.7° [26]. This narrowing of the jet spreading angle is due to the limited mass available for the jet to entrain, resulting in ‘self-entrainment’ which effectively narrows the spreading angle of the jet. Analogous to the
equation derived for a free jet, knowledge of the jet spreading angle allows derivation of an expression for the axial location at which the confined jet extends to the wall (again, $L$ is reactor radius) and consequently the recirculation zone ends:

$$X_P = 5.85L$$ (3-4)

Beer and Chigier [25] note that the Thring-Newby criterion (which states that jet spread is due to shear induced entrainment for either free jets or confined jets) under which this equation is derived provides good agreement with experimental data when the nozzle diameter is smaller than 1/10 of the duct diameter, which is true for this work ($d/D = 0.039$). Comparable to turbulent free jets, similarity is implied between turbulent confined jets with vastly differing parameters. This is illustrated in Figure 3-5 which shows similar relative flow profiles for different inlet velocity and reactor pressure conditions. Regardless of velocity or flow rate, two turbulent confined jets inside the same size enclosure are theoretically predicted to have the same recirculation zone length. Equation 3-5 also implies that the recirculation zone length is a function only of the confining geometry and not the jet diameter (assuming that the jet diameter is sufficiently small compared to the confining geometry, i.e., 1/10 of the duct diameter).
Figure 3-5: A vertical contour plot of axial velocity for the 20 bar baseline and 5 bar cases of this study. Note the velocity magnitude differences between cases.

Brief consideration for the case in which secondary flow is introduced alongside the core jet should also be addressed here as it is applicable to this work. Figure 3-6 illustrates free jet entrainment behavior, confined jet entrainment behavior with no secondary mass flow, and confined jet entrainment behavior with some secondary mass flow. Two conditions exist for a confined jet with secondary flow, those in which there is insufficient secondary mass flow (including zero secondary mass flow) to support free jet entrainment such that a recirculation zone is setup, and those where sufficient secondary mass flow is introduced with negligible momentum to preclude the development of a recirculation zone. The bottom illustration in Figure 3-6 shows the insufficient secondary mass flow condition.
Figure 3-6: A qualitative flow field visualization for a free and confined turbulent jet without and with secondary mass flow. Note the recirculation zones that develop in the near burner region close to the jet origin. Point P represents the point where the jet boundary impinges on the wall. $X_P$ represents the axial location at which the jet spreads to the reactor radius $L$. A free jet would reach radius $L$ at a shorter axial distance compared to a confined jet due to the lack of a recirculation zone from self-entrainment. Figure(s) from Barchilon and Curtet [30].

The term ‘sufficient’ here means a quantity of mass flow that would allow the jet to entrain exactly as a free jet would without being affected by the enclosing walls (Figure 3-6). In the case where sufficient secondary mass is supplied, the jet will spread like a free jet and reach the enclosing walls at an axial position of $4.5L$ rather than $5.85L$. When there is insufficient secondary mass the jet will attach at an axial position of $5.85L$. The amount of secondary mass flow needed to avoid recirculation can be calculated using the following equation from Ricou and Spalding [31]:

Free Jet

$$X_P = 4.5L$$

Confined Jet: No secondary mass flow

$$X_P = 5.85L$$

Confined Jet: Secondary mass flow

$$X_P = 4.5L \quad 5.85L$$
\[
\frac{m_x}{m_o} = 0.32 \left( \frac{\rho_e}{\rho_o} \right)^{0.5} \frac{x}{d_j}
\]  

(3-6)

where \(m_x\) is the mass flow rate of the jet at some axial position \(x\), \(m_o\) is the initial jet flowrate, \(\frac{\rho_e}{\rho_o}\) represents the ratio of the environment density to the jet’s initial density, and \(d_j\) is the jet diameter. The lack of a recirculation zone would allow for an even greater computational speedup using a DA mesh because only the axisymmetry requirement would need to be met before transition to the axisymmetric computational domain could be performed. For the primary flowrate used in this work, a secondary mass flowrate \(~18.5\) times greater than the center jet flow rate would be necessary to avoid the setup of a recirculation zone. Since the secondary mass flowrate in this work was only \(1.8x\) the primary flowrate, it had a negligible effect on the recirculation zone length. That is to say, the center jet behaved as a confined jet across all studies performed and attachment was observed at an axial position near \(5.85L\) (as will be shown in the Results section).

Ultimately, it has been shown that for the geometry of interest (cylindrical combustors), that recirculation zones are the limiting factor in the placement of the dimensional boundary and that recirculation zone length is a function only of the confining geometry. This then means that for a wide variety of operating conditions the dimensional boundary can be placed at the same axial location with confidence that all conditions requisite at the boundary will be met. One caveat should be noted here, these conclusions are valid for a dimensional boundary that decouples the 3D and axisymmetric domains. If the dimensional boundary were to be made to accommodate two-way (elliptic) flow, then recirculation zone length would no longer play a role in the dimensional boundary placement and the only constraint on boundary placement would be the flow development length.
4 RESULTS AND DISCUSSION

4.1 General Information

Once CEDAR was completed a series of studies were undertaken to examine the effects various operating conditions had on the flow field as well as to evaluate the accuracy of DA meshing when compared with fully 3D results. These include:

- Application 1: Pipe Flow
  - Runtime Dependence on Boundary Location for a Pipe Flow

- Application 2: POC
  - Parametric Study of Pressure Variation
  - Parametric Study of Firing Rate
  - Runtime Dependence on 3D Domain Symmetries

The Baseline case of this study is based on the POC geometry, that is, a down-fired cylindrical reactor with a central primary jet and tangentially periodic secondary inlets (see Figure 4-1 and Figure 2-1). The reactor diameter is 0.2032 m and length is 1.5 m with a fully open outlet. The primary inlet mass flow rate is 7.81E-3 kg/s. The total secondary flow rate over all inlets is 1.493E-2 kg/s. The operating pressure is 20 bar, meaning the full reactor is operating at a pressure of 20 bar. These flow rates are based on typical operating conditions for a firing rate of 100 kWt in the reactor. Uniform velocity profiles are prescribed based on continuity
at both the primary and secondary inlets. All runtime dependence and parametric studies are some variation of this Baseline. For example, all the cases in the parametric pressure study utilized the above-mentioned flow rates but varied pressure from case to case. All other parameters were kept constant unless otherwise noted. Under relaxation values for all cases are 0.75 except for the pressure and pressure correction factors which were set at 0.94 and 0.98 respectively. All cases were converged to a maximum residual value of 3.5E-4. This maximum residual value was determined based on a sensitivity study using a fixed geometry and mesh. The sensitivity parameter used was the exit velocity profile. The maximum residual value was incrementally decreased until the predicted profile variance was less than 1%. The residuals calculated and monitored include all three velocity components, mass, pressure, turbulent kinetic energy, turbulent eddy dissipation, gas mixture fraction, and gas mixture fraction variance.

**Figure 4-1:** A contour plot just downstream of the reactor inlets showcasing their locations inside the POC reactor. One half of the symmetric reactor is shown in this case. Note the primary center jet (red) and four tangentially periodic secondary inlets (yellow/green).
All cases were run in serial on a Windows computer with an Intel® Core™ i5-6500 CPU at 3.2 GHz and 32 GB RAM.

4.2 Runtime Dependence on Boundary Location for a Pipe Flow

The Pipe Flow cases were all conducted on a 130 x 60 x 60 (X x Y x Z) node mesh at a Re = 200,000 in a 0.2032-m diameter pipe that was 1.5 m long. Fully developed pipe flow is itself an axisymmetric flow. After its completion, CEDAR was used to evaluate a pipe flow to assess its ability to accurately represent a known axisymmetric flow. The axisymmetry of the flow allowed the placement of the boundary virtually anywhere within the computational domain. This presented an opportunity to characterize the reduction in computational time as a function of the position of the dimensional boundary as is shown in Figure 4-2 below.

![Figure 4-2](image_url): A non-dimensionalized plot of computational time as a function of the position of the dimensional boundary within the computational domain.

\[ y = 1.166x^2 - 0.1858x + 0.0134 \]

\[ R^2 = 0.9997 \]
As the dimensional boundary is moved upstream (i.e., the 3D domain is reduced) the time required to achieve solution drops quadratically with the number of computational cells. This suggests that if even a small portion of the entire computational domain can be accurately characterized as axisymmetric, then significant time savings are possible using a DA mesh. For example, with the dimensional boundary placed at an \( x/L = 0.5 \), the DA mesh computations would be expected to take \( \sim 20\% \) of the time of a fully 3D mesh computation.

Comparison of the exit axial velocity profiles over the radius of the pipe can be seen in Figure 4-3. Generally, the DA mesh results are very comparable to the fully 3D profile. All the DA mesh results shown here appear to over predict the velocity near the wall and under predict it in the bulk flow toward the center of the pipe. Difference in centerline outlet velocity (at \( R = 0 \)) for fully 3D predictions are 3-5% greater than DA cases. This result shows that for a wide range of dimensional boundary locations, CEDAR can consistently provide physically realistic results while using a DA mesh.

![Figure 4-3](image)

**Figure 4-3:** Predicted radial profiles of axial velocity at the exit of the pipe for several of the pipe study cases with modified dimensional boundary location.
4.3 Parametric Study of Pressure Variation

The pressure study is composed of six cases, three fully 3D cases and their corresponding DA counterparts. A half symmetry of the Baseline case was simulated for all cases in this study on a 130 x 61 x 120 node mesh. Three different operating pressures of 5, 10, and 20 bar (i.e., system pressures) were used for this study. Mass flow rates for all cases are the same as the Baseline case. Because of this, as pressure was decreased from 20 to 5 bar, inlet velocities had to increase 4-fold to maintain flow rates. This variation in operating pressure and inlet velocities was expected to produce a large difference in the resultant flow field. However, this is not what was observed in simulation results.

The results pictured in Figure 4-4 and Figure 4-5 show that the resultant flow structure over all cases is extremely similar in spite of the large differences in operating pressure and velocity. Note the dashed red lines in Figure 4-5 indicating the observed reattachment point of the recirculation zone (0.61m) which agrees favorably with the 0.594 m predicted by Equation 3-4. For all cases the flow in the near burner region is composed of a strongly downward flow from the primary jet, and a strong upward flow attributed to the entrainment of mass by the central jet as it progresses down the reactor. The entrainment of secondary fluid at the central jet boundaries leads to a low pressure region in the near wall region of the reactor which then draws in fluid from downstream to replace that entrained by the central jet, resulting in recirculating flow in the approximately first 0.23 m of the reactor. Additionally, the central jet is seen to spread at an approximately linear rate until ~ 0.2 m at which point it begins to balloon radially outward and axial velocity decreases sharply. This behavior is explained best by viewing normalized pressure contours (see Figure 4-6).
**Figure 4-4:** Contour plots of normalized axial velocity inside the POC Reactor for the Pressure Study. Note that the reactor centerline is located at $R = 0.1016 \text{ m}$ in these figures.

**Figure 4-5:** A tighter scale view of the normalized axial velocity inside the POC Reactor. Note the similarity in flow structure over the range of pressures used in this study. The dashed red line indicates the observed recirculation zone length (0.61 m). The reactor centerline is located at $R = 0.1016 \text{ m}$ in these figures.
Figure 4-6: Pressure contour plots for each of the pressures examined in the pressure study.

The pressure profile in the reactor generally shows increasing pressure as the flow progresses axially down the reactor. This result agrees with that predicted by conservation of linear momentum. A control volume analysis (neglecting the effects of drag [32]) in which the downstream control surface is chosen such that it is beyond the axial location at which the jet impinges on the reactor walls yields the following equation:

$$\frac{\Delta p}{\rho U_j^2} = \left(\frac{A_j}{A}\right)^2 = \left(\frac{d_j}{D}\right)^2$$

(4-1)

Where $\Delta p = p_2 - p_1$, subscript $j$ refers to the inlet jet, $A$ is cross sectional area, $D$ the container diameter, $d$ the jet diameter, and $U$ the axial velocity. This equation indicates that $\Delta p$ must be greater than zero moving axially down the reactor. Note also that the pressure rise from the inlet (point 1) to the exit of the control volume (point 2) is directly proportional to the square of the ratio of jet cross section to reactor cross section, or equivalently, the respective diameters. Thus, for a fixed geometry, the magnitude of pressure rise observed should scale with the square of the
jet inlet velocity. The pressure rise required by conservation of momentum also acts to alter the jet shape. Instead of spreading linearly to the wall the jet takes on a ‘bell shape’ as can be seen in Figure 4-5. Of interest as well is the magnitude of the far field velocity. Due to the high pressures the bulk flow velocities are small; especially compared with those of an air-fired reactor of the same geometry and firing rate. This translates to low global Reynolds numbers for the flow (~10,000). Consequently, even though the flow is turbulent, outside of the near burner region the flow is quite slow and the gradients are small. This kind of flow is seen to make up a large portion of the computational domain. This suggests that significant computational resource is being used to resolve a flow that largely does not need such resolution, and that a dimensionally reduced mesh could be appropriate in these regions.

To assess the benefits of using DA mesh, the three pressure cases were run using DA meshes and compared to the fully 3D (half symmetry) simulations. Timing results are shown in Figure 4-7 for all six cases run as part of the Pressure Variation study. The dimensional boundary was placed 0.701 m from the burner inlet for each of the DA cases. Note this is similar to but slightly downstream of the 0.6 m recirculation reattachment point suggested by Equation 3-4, and allows for some margin of error with the discrete computational cell sizes. The average speedup obtained over all cases was 4.76. Recall that for the Domain Symmetry study the greatest speedup was 4.26 times, thus the DA mesh provided a 10% speedup over a simplified geometry approach. In addition to this speedup, a DA mesh retains the ability to simulate non-periodic burner designs as opposed to a simplified geometry approach which can only be used with periodic designs. Furthermore, in cases where an even greater portion of the computational domain can be approximated as axisymmetric, greater time savings can be expected from a DA
meshing approach. Note also that this is within 14% of the predicted speedup for the Pipe Flow case for an axial location of $x/L = 0.467$ (see Figure 4-2).

**Figure 4-7:** Timing results for the Pressure Variation study comparing 3D meshes with DA meshes (DA boundary at 0.701 m).

For all pressures, the resultant radial exit velocity profiles (shown in Figure 4-8) predicted by the DA mesh are on average within 1.5% of fully 3D profiles, with no greater than a 5% difference at any single radial position observed. This result shows that with a properly placed dimensional boundary, DA meshing can produce very comparable results to a fully 3D mesh at a considerably reduced computational time, and that reduced computational times are consistent across all pressure conditions.
Figure 4-8: Comparison of 3D and DA mesh axial velocity profiles at the exit of the POC reactor for pressures: (a) 20 bar, (b) 10 bar, (c) 5 bar.
Figure 4-8 (continued): Comparison of 3D and DA mesh axial velocity profiles at the exit of the POC reactor for pressures: (a) 20 bar, (b) 10 bar, (c) 5 bar.

4.4 Parametric Study of Firing Rate

Like the Pressure Variation study the Firing Rate study is comprised of six cases. Three fully 3D cases and three DA cases. Again here the geometry used was a half symmetry of the Baseline case on a 130 x 31 x 60 node structured mesh for each case in the study. Part of the motivation in conducting this study was to further examine the flow similarity observed in the Pressure Variation study to see if it would persist when the flow rates (and therefore Reynolds numbers) of the jets were changed. Pressure was held constant at 20 Bar for all cases. Three firing rates were utilized, namely 50, 75 and 100% of Baseline. Reduction in firing rate was represented as a linear reduction in inlet mass flow rate (or inlet velocities for similar density flows). Varying flow rates allowed for a stronger test of similarity due not only to velocities changing but the jet Reynolds numbered being varied simultaneously.
Figure 4-9: Axial velocity contour plots for the three Firing Rate cases examined in this study. Similarity of the flow is maintained even when jet Reynolds numbers are varied.

Figure 4-10: A tighter scale view of the normalized axial velocity field for the Firing Rate cases. Note again the ‘ballooning’ out of the center jet beginning at ~ 0.2 m.
Flow similarity is still observed across all three cases, even when the inlet jet Reynolds numbers are varied (all Rej in this work are turbulent). Thus it can be concluded that flow field similarity can be expected for cylindrical down-fired combustors with a central jet even with discrete tangential secondary flow inlets, provided the inlet jets are sufficiently turbulent and the individual secondary inlet momenta are negligible compared to the center jet. This conclusion means that for a wide range of operating conditions (both flow rate and pressure as shown in this work) the flow field structure can be expected to remain largely invariant, other than its magnitude. It also implies that a single simulation can provide an accurate description of conditions inside the reactor for a wide range of steady state operating conditions. The DA meshing approach used here also allows for changes in the burner design (which consequently changes the 3D flow field near the burner), without affecting the reattachment correlation, i.e., the placement of the dimensional boundary.

Timing results for the Firing Rate study (Figure 4-11) are similar to those from the Pressure Variation study. A significant speedup was achieved when using a DA mesh over a 3D mesh. In this study the average speedup was 5.56 times. This is notably higher than the average speedup of 4.76 times observed in the Pressure Variation study. This difference in relative speedup is in part attributed to the different meshes utilized in each respective study. The Pressure study utilized the ‘fine’ mesh (130 x 61 x 120) with significantly more computational nodes, while the Firing rate study was conducted on the ‘coarse’ mesh (130 x 31 x 60). In general, two main factors have an influence on the speedup possible with a DA mesh. The first is the reduced dimensionality of the flow. This manifests itself algorithmically as a reduction in the total number of computations per node (in the axisymmetric domain) required for solution (i.e. 4 neighbors rather than 6). The other factor being a reduction in total number of
computational nodes with a DA mesh. The total reduction being on the order of the product of the corresponding numbers of axial and tangential cells in a fully 3D mesh that occupy the same positions as the axisymmetric portion of the DA mesh.

Figure 4-11: Timing results of the Firing Rate study comparing 3D meshes with DA meshes (DA boundary at 0.701 m). DA meshing provides a consistent speedup over its 3D counterpart.

Exit velocity profile predictions for the Firing Rate cases are shown in Figure 4-12. All DA mesh results show good agreement with the fully 3D mesh profiles. The average error for all cases in the Firing rate study is below 5%. The largest errors are again observed to occur near the wall, just as in the Pressure Variation study. The larger difference observed in this study is attributed to the coarser mesh spacing used here relative to the Pressure Variation study. The wall of the physical reactor is a continuous, smooth curve, which is approximated as a discrete, discontinuous profile in the Cartesian 3D mesh. As mesh size is reduced this approximation is expected to become a more accurate representation of the physical system. This is confirmed by the smaller relative error in near wall predictions as shown in Figure 4-8.
Figure 4-12: Exit axial velocity profile comparisons between fully 3D and DA meshes at various Firing Rates: (a) 1.0 (100%), (b) 0.75 (75%), and (c) 0.50 (50%).
Figure 4-12 (continued): Exit axial velocity profile comparisons between fully 3D and DA meshes at various Firing Rates: (a) 1.0 (100%), (b) 0.75 (75%), and (c) 0.50 (50%).

4.5 Runtime Dependence on 3D Domain Symmetries

The objective of this geometry study was to explore the viability and practicality of taking advantage of the periodic symmetry of the POC reactor (i.e., the Baseline case geometry). This is a common modeling approach used in industry to reduce computational time. The purpose of including this type of study in this work was to allow for a representative comparison of the speedup and accuracy tradeoffs between simplified geometry and DA meshing for the same geometry. This study consisted of three cases: full Baseline case geometry, half Baseline case geometry, and a quarter Baseline case geometry. The timing results for each case are shown in Figure 4-13.
Figure 4-13: Timing results for the three cases of the Geometry Study. The computational time decreased quadratically with cell number, similar to the DA cases.

It becomes clear why this method is used so often after seeing the results of the timing study. The half symmetry or half geometry case is 2.6 times faster while the quarter symmetry case is approximately 4.3 times faster than the fully 3D case with no appreciable loss in accuracy when using the exit velocity profile as the metric for measuring accuracy. Axial velocity profiles for these three cases are shown in Figure 4-14.

Both the half symmetry and quarter symmetry exit velocity profiles vary less than 2\% from the fully 3D results. The combination of speed up and small accuracy loss at the exit highlight why this approach is widely used in industry.
Figure 4-14: Exit axial velocity profiles as a function of reactor radius for three domain symmetries (full geometry, half symmetry, quarter symmetry).

The above results are comparable to those from using a DA mesh, including the quadratic reduction with computational time with reduction in computational cells. However, the DA approach is approximately 10% faster than domain symmetry with comparable accuracy (3-5%). The DA technique also maintains the advantage of being able to accommodate more general geometry, in this case meaning non-periodic inlet designs. Additionally, even greater speedups can be expected with the DA technique as the dimensional boundary is moved higher (smaller 3D region) within the computational domain.
This work developed and assessed use of a Dimensionally Adaptive (DA) meshing technique to help speed the solution of a non-reacting pressurized fluid flow in a cylindrical geometry with non-axisymmetric inlet flow conditions. A DA-capable code, CEDAR, with an \textit{a priori} dimensional boundary locator was developed based on extension of previous 3D RANS flow solvers. Assessment of the technique was based on the CEDAR’s ability to reproduce fully 3D exit velocity profiles and the time required to do so. The approach used to accomplish this consisted of five main research tasks: (1) Develop or obtain source code for a 3D turbulent flow solver. (2) Validate the 3D turbulent flow solver using published jet profile data. (3) Modify the validated flow solver to accommodate DA meshes. (4) Compare DA calculation accuracy and computational time with the validated fully 3D results. (5) Develop a dimensional boundary locator algorithm based on non-reacting jet theory correlations.

The structure of the 3D solver was largely based on two codes previously developed at BYU (PCGC3, and gas3D). It was ported from FORTRAN into PYTHON in anticipation of its later integration as part of a larger comprehensive CFD tool. Initial evaluation of the solver once porting and development was completed revealed that the PYTHON version of the solver was significantly slower than the equivalent FORTRAN code. This issue was resolved by employing
the use of the NUMBA JIT compiler which resulted in an ~300% reduction in the runtime of the solver, bringing it back on par with C and FORTRAN code speeds.

First it was shown that the solver could provide physically realistic results over a large range of Reynolds numbers by comparing the velocity profiles produced by the solver for pipe flows at Reynolds numbers of 20 and 200,000, respectively, with those predicted by theory. Next the solver results were compared with LDA data for a central axis down-fired non-reacting flow. Good agreement was observed with the measured data. The recirculation zone length was observed to be slightly under predicted when compared with measurements. However, the spreading behavior and recirculation in the near burner region were both correctly reproduced.

The general considerations for DA meshing for fluid flow were discussed. For cylindrical combustors with large length to diameter ratios, the flow will eventually become axisymmetric. At this point the tangential derivative terms in the governing equations can be dropped with minimal accuracy loss. The dimensional boundary was then considered. The dimensional boundary as currently implemented in CEDAR decouples the 3D and axisymmetric domains. One-way, axisymmetric flow is assumed at the dimensional boundary. Placing it at a location in the computational domain that violates either of these assumptions provides no guarantee of physically realistic results.

CEDAR requires that the dimensional boundary be located at a point in the computational domain where the flow is both one-way and axisymmetric. It was found that the flow becomes axisymmetric at ~0.3-0.4 m for the geometry and burner design considered in this work. Recirculation zone length was found to be the limiting factor in the placement of the dimensional boundary as the recirculation zones were found to extend beyond the 0.3-0.4 m range to approximately 0.61 m. With good agreement free and confined jet theory were then
used to predict the recirculation zone length within the reactor. Theory suggests that this length is independent of Reynolds number and jet diameter (assuming the jet to be < 1/10 the diameter of its confining geometry) for any jet, and is only a function of the confining geometry’s diameter. Thus the dimensional boundary locator is a simple linear function of the radius of the reactor and may be expressed as $5.85L$ where $L$ is the reactor radius.

Several studies were undertaken to examine the effects of varying operating conditions on the resultant flow field solution, as well as to evaluate the ability of CEDAR to accurately reproduce fully 3D results. Timings of all cases were conducted to compare the relative speedup achieved using DA meshing. Generally, exit velocity profiles over all studies deviated less than 5% from fully 3D results. With the dimensional boundary placed 0.701 m from the inlet in a 1.5-m long reactor resulted in an average speed up of 5.16 times over fully 3D simulations. This shows that DA meshing can both quickly and accurately resolve the flow field in cylindrical geometries with large length to diameter ratios for a wide range of operating conditions.

The current approach for DA meshing in CEDAR decouples the 3D and axisymmetric domains. Future work could develop a 2-way dimensional boundary, that would allow for information exchange between dimensional domains. This could potentially lead to even larger speedups because the current requirement for the flow to be one-way at the boundary would no longer be necessary. Additionally, active mesh refinement techniques could be incorporated into CEDAR, thereby allowing the dimensional boundary position to be actively moved during simulation. Lastly a sensitivity study could be undertaken to examine which flow variable is most sensitive to the placement of the dimensional boundary as well as any differences in the upstream (3D) flow field solutions’ sensitivity to the dimensional boundary position.
REFERENCES


