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RPPR Final Report
as of 09-Nov-2018

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STEM Degrees: 2 **STEM Participants:** 2

Major Goals: The overriding goal, the real objective of the current proposal, is to develop a three-dimensional unsteady numerical model that can be used to simulate the unsteady behavior of fire whirls. The model must be capable of simulating the dynamics of the transition between fire whirls and the blue whirl. There were three major goals in the project that contribute to the overall objective: 1. Test the basic fluid algorithm for solving the unsteady, compressible Navier-Stokes equations by predicting vortex breakdown in the same general regime of temperature and pressure as the blue whirl. 2. Develop a calibrated, simplified chemical-diffusive model (CDM) for heptane-air vapor combustion. The model should cover a range of equivalence ratios from fuel-lean to fuel-rich conditions. 3. Produce a first-pass simulation for conditions that might evolve into a blue whirl. Coordinate this with ongoing experiments at ARL Adelphi and the University of Maryland.

Accomplishments: The accomplishments of the program were generally aligned with the goals. We therefore:
1. Tested the basic fluid algorithm for solving the unsteady, compressible Navier-Stokes Equations in the same regime of temperature and pressure as we expect to see a fire whirl than transitions to a blue whirl. For this, we tested the standard explicit computation, and then began the conversion to a low-mach-number version which would be affordable. The test problem was computation of vortex breakdown. We now now tested models that are affordable for high-speed and low-speed flow.
2. Developed and begun the calibrated, of a simplified chemical-diffusive (CDM) model for heptane-air vapor combustion. The model should cover a range of dilutions from fuel-lean to fuel-rich conditions. The diffusion flame model is being tested and calibrated now.
3. Produced a first-pass simulation for conditions that might evolve into a blue whirl. This entire project is well-coordinated this with ongoing experiments at ARL Adelphi and at the University of Maryland..

Training Opportunities: This project offered in-depth training in computational physics and computational fluid dynamics to two graduate students working at the University of Maryland, Ms. Xiao Zhang and Mr. Joseph Chung. They simultaneously took courses in Aerospace Engineering and Fire Protection Engineering at the University of Maryland.

Results Dissemination: The discovery of the blue whirl went "viral" in the media about a year ago. It was covered in all major news outlets, including the New York Times, Science, American Scientist, and so forth. As a result, we continue to get enquiries from students and researchers all over the world, and we also continue to get visitors from elementary schools through research laboratories. There is a continual flow through.
Most of the visitors want to see experiments, but we also show them the incipient computations and try to stress how difficult it is to do these, and how we must have these computations in order to explain the phenomenon.

RPPR Final Report
as of 09-Nov-2018

Honors and Awards: Elaine Oran -- Elected Fellow, American Academy of Arts and Sciences
Elaine Oran -- Elected Fellow, Combustion Institute
Appointed to inaugural A. James Clark Distinguished Chair in Aerospace Engineering,
University of Maryland

Protocol Activity Status:

Technology Transfer: DoD interactions were with
1) ARL Adelphi, the group headed by Dr. Ivan Lee, who is carrying out relevant experiments.
2) Naval Research Laboratory (NRL) discussions with Dr. Gabriel Goodwin.

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Project Contribution:
International Collaboration:
International Travel:
National Academy Member: Y
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International Collaboration:
International Travel:
National Academy Member: N
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Participant Type: Graduate Student (research assistant)
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Person Months Worked: 4.00 **Funding Support:**
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International Travel:
National Academy Member: N
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Other Collaborators:

RPPR Final Report
as of 09-Nov-2018

Final Report for the STIR Program

Numerical Simulation of the Blue Whirl

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Numerical Simulation of the Blue Whirl

Final Report

Introduction

The blue whirl is a flame structure that was originally observed when it evolved *naturally* from a (relatively) small fire whirl burning liquid heptane. It was produced serendipitously in a laboratory setting during a study to evaluate the burning efficiency of fire whirls [1]. Once formed, the blue whirl remained in the steady, stable, completely blue state, forming no soot at all, until all of the fuel was consumed.

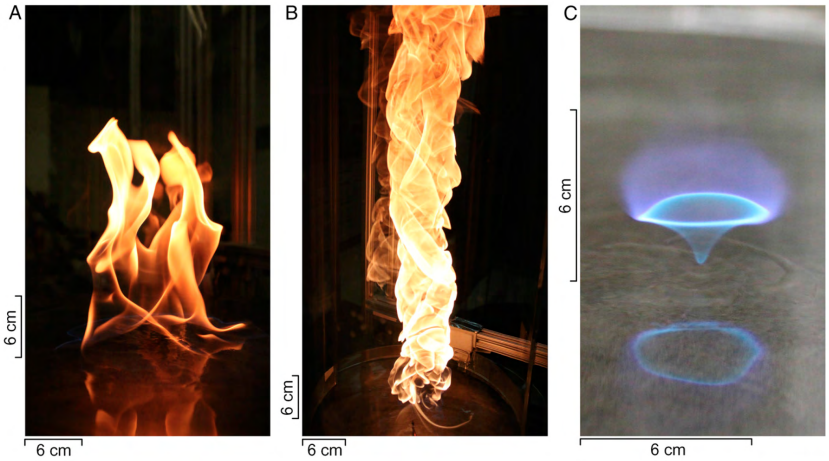

Figure 1. Evolution from a pool fire to a blue whirl over water. (A) Pool fire forms following ignition. (B) Canonical fire whirl develops subsequent to the pool fire. (C) Previously unobserved laminar blue whirl evolves from the yellow fire whirl. The vertical scale marked on the side of each image starts at the water surface. Figure taken from [1].

After the blue-whirl flame state was discovered, it became a topic of curiosity and controversy in the combustion community. It was a curiosity to theoreticians because it appeared to be a self-sustaining flame with an unknown structure, and it became an opportunity for combustion engineers because it burned liquid hydrocarbons without producing any soot. Further experiments told more about its structure and dynamics [2, 3], but these raised even more questions. Could it scale to a much larger size? Is it possible for a blue whirl to form directly without having to go through a fire-whirl stage? What causes the transition from a fire whirl to a blue whirl? How is it related to fire whirls? And perhaps most curiously, why was it not seen before? Experiments are difficult and dangerous to perform, and so new results came forth relatively slowly.

The general consensus was that we need a numerical simulation of a fire whirl and use it to study the transitions to a blue whirl. Such a capability would be useful for structuring and guiding future experiments and applications. In addition to interpreting the structure and evolution of the blue whirl, the simulations could be used in the future to extend the experiments and analysis to other flow regimes to address issues of stability, scaling, and transition mechanisms.

The primary objective of this proposal was to begin the process of creating a numerical model that would be capable of simulating the observed liquid-fueled fire whirl and its evolution to a blue

whirl. Once we have such a tool, it could be used in subsequent projects, and in close conjunction with ongoing experiments at the University of Maryland, in the laboratory of Dr. Michael Gollner, and at ARL Adelphi, in the laboratory of Dr. Ivan Lee, to interpret and guide the experiments. Dr. Lee is supported under the ARL Director's Research Award (DIRA) Transformative Research Challenge (TRC) program.

Over the past forty years, we developed many unsteady, multidimensional numerical simulation models for reactive flows and have used these to solve problems ranging from premixed flames to diffusion flames, including complex reactions ranging from chemical to nuclear, with applications ranging from engine combustion to astrophysics. The blue whirl presents a particular challenge for two reasons. First, the phenomenon is fully three-dimensional and there are no short cuts in doing lower-dimensional analyses. Second, the chemical reaction in the original problem was for a complex hydrocarbon fuel, and a reaction model for whatever fuel is burned must represent a wide range of equivalence ratios, from pure fuel in a liquid state through to a fully reacted fuel-air mixture at varying equivalence ratios. As the project proceeded, we discovered other difficulties to overcome, and these are described in the material in this report.

The general direction and management of the project was carried out by Dr. Elaine Oran, who has had extensive experience developing a wide range of combustion and reactive-flow models, ranging from laminar to turbulent flows at creeping through hypersonic velocities. Dr. Carolyn Kaplan, who has expertise in multidimensional, unsteady combustion simulations, and, in particular, of including detailed chemical and soot models in simulations of diffusion flames, was the Co-PI and the primary person directing the implementation of chemical models. This research is the basis for doctoral research of two graduate students, Mr. Joseph Chung and Ms. Xiao Zhang. Both of these students have their masters degrees, are enrolled in the Ph.D. program at the University of Maryland, and have experience now with the types of fluid and reactive flow codes needed for this project. The needed additional funding was obtained from the Minta Martin Endowment Funds from the Department of Aerospace Engineering and through the Glenn L. Martin Institute Chaired Professorship at the A. James Clark School of Engineering.

Extensive computations were performed using the University of Maryland Deepthought2 HPC cluster and the Air Force Research Laboratory's Thunder. We are grateful to the Laboratory of Computational Physics, Naval Research Laboratory (NRL), for providing the DoD supercomputing resources to access Thunder to Mr. Joseph Chung.

The proposed work for the STIR proceeded systematically with simultaneous development and testing of a new fluid dynamics algorithm and submodels for the most relevant chemical and physical processes. The results, as described in this report, are a three-dimensional (3D) unsteady fluid model that demonstrated vortex breakdown, a new calibrated chemical model for heptane combustion, and a preliminary simulation of a fire whirl.

Background and Perspectives

This section is an interlude inserted to provide motivation for the eventual problem we wish to solve. Here we address this question: What is the blue whirl, and why is it intriguing and surprising to the general combustion community. To do this, we first list characteristics of the blue whirl that have been determined from laboratory experiments. These were carried out at UMD [1, 2, 3], and

experiments are currently also being carried out and expanded by work at other laboratories, such as ARL Adelphi and some at the University of California San Diego (UCSD).

The reported measurements and observations were made for a relatively simple experimental configuration consisting of two offset half cylinders. The gap between the cylinders allows air to be entrained at whatever rate occurs naturally. Fuel is poured or injected onto a water or other surface and then lit. A pool fire develops first, but this usually transitions quickly to a fire whirl. At some point, this fire whirl transitions into a blue whirl. The three stages are shown in Figure 1.

Below is a summary of the observations. Some interpretation or additional comments are indented under the observations.

1. The blue whirl evolves *naturally* from an intense fire whirl formed by burning a liquid hydrocarbon on water. This was originally reported in experiments at UMD [1, 2, 3], and later the experiment was partially repeated at Princeton University in the laboratory of Alexander Smits and Katie Hartl. Subsequently it was seen in ARL Adelphi by Ivan Lee and Paul Anderson, and also at the University of California San Diego by Antonio Sanchez and Wil Coenen.
   - From these, we see that the transition to a blue whirl does not depend on the general shape of the enclosure. It can be produced in round enclosures and square enclosures. Recent observations of naturally occurring fire whirls might suggest that blue whirls could appear in unconfined scenarios and at larger sizes.
2. The blue whirl can be described as a spinning blue top, which is brightest blue around the top ring. (See Figure 1C.)
   - There is a commercial spinning top that can be purchased, ForeverSpin, that claims to have achieved the ideal shape for stable spin. Its shape is looks very much like the blue whirl.
   - The blue color *suggests* that this corresponds to a well mixed (premixed) flame. This is discussed more below.
3. There is a hat or cone on top of the spinning top that is a faint purple with a touch of green. This can be seen in Figure 1C.
4. Measurements [2, 3] show that the temperature inside the violet haze is 2000 K.
   - The temperature of 2000 K in the violet haze is much higher than obtained in a normal diffusion flame and closer to that in a premixed flame. It is not yet known for certain if there is burning in this region or whether it is a bath of hot products.
   - These measurements also confirm that the temperature is too low for soot formation in the ring, which is less than 1700 K, in the blue region.
   - In the high-temperature region, the 2000 K violet region above the blue ring, there is also no soot.
5. Once the blue whirl forms, the noisy turbulent fire whirl, shown in Figure 1B, disappears. The small spinning blue whirl is quiet and moves around slightly above the surface.
   - There appears to be no turbulence in the blue whirl. Nothing external is changed purposely or driven externally any differently to create the transition.
6. When the blue whirl becomes unstable, yellow-orange flames appear in the center of the blue whirl. The spinning blue ring persists, but these yellow-orange flames, which seem to have structures typical of vortex-breakdown modes, appear in the center. After a few seconds, these

structures disappear from view and only the blue whirl remains. A typical unstable sequence is discussed in detail in [1].
   - When the blue whirl becomes unstable for short periods of time, we see soot forming in the central region and extending upwards. If we can consider the soot as a flow diagnostic, it appears that the flame is undergoing a number of mode transitions characteristic of vortex breakdown. We also see these modes appearing when the initial, sooty fire whirl transitions to a blue whirl. This could be a key to the transition and will be discussed more in a later section of this report.
7. Blue whirls were created from a fire whirl using a range of hydrocarbon fuels, including heptane, octane, crude oil, and fortified rye whiskey [2, 3].
8. Once the blue whirl forms and is stable, it burns until all of the spilled fuel is removed from the surface. If the fuel is fed to the surface from below, the blue whirl persists until the reservoir is emptied.
9. The blue whirl can also be formed from a fire whirl created by a fuel spill on a smooth metal surface. If the surface is too porous, it cannot be stabilized.
   - That the blue whirl appears on a water surface or on a smooth metal surface suggests that a smooth boundary is important. Recent experiments [4] have shown that if the inflow into the chamber is smooth (less turbulent), the blue whirl forms more easily and stably.
10. A gas burner using propane is now being used to try to create a blue whirl.
    - This configuration produced an unstable blue whirl. It looks promising.
11. Very recent experiments [4] have put the blue whirl on a fire-whirl diagram of circulation vs energy release. These results indicate that the blue whirl is in a near-limit fire-whirl regime.
    - Recent attempts to go directly to a blue whirl and bypass the fire whirl have not yet succeeded (private communication, Yu Hu). There are ongoing attempts to do this, however.

In summary, we have seen in laboratory experiments that the blue whirl naturally burns heavy liquid hydrocarbons, without any atomization or moving parts, and without producing soot. The blue whirl is laminar. It starts from a *self-induced vortex*, and it appears when there is vortex breakdown in the fire whirl. Vortex breakdown in a fire whirl is an effect that up to now has been suggested, and this suggestion has been repeated in the literature, but it has not been definitively demonstrated before. The chemical and physical structure of the blue whirl are uncertain. The mechanism of transition might be the result of vortex breakdown, but it has not been proven.

Here are some intriguing questions and problems related to the blue whirl:
- Can we construct a robust combustor that will burn any hydrocarbon fuel with no soot, minimal pollution, and no need for fuel atomization?
- What is the chemical structure of the blue whirl? Is it a combination of premixed stoichiometric, lean and rich burning occurring in various portions of the flame? Are all of the blue regions triple flames, as has been conjectured? Is there burning in the central, violet portion? Why is the temperature so high?
- Does the blue whirl scale? Can we make a large one?
- Is it necessary to go through a normal fire whirl stage in order to transition to the blue whirl? Are there other, less dramatic and dangerous ways to form it?

– What triggers the transition from a fire whirl to a blue whirl? Is vortex breakdown important in this process? We have speculated that the blue whirl is a bubble-type vortex, and the usual fire whirl consists of changing combinations of bubble, helical, and spiral modes. We might, in fact, hypothesize that the lower blue region of the blue whirl could be the lower portion of a bubble, and part of the upper violet regions could be part of the upper portion of the bubble. The blue whirl then would correspond to an intense, reactive bubble mode. Now as we see below, all of this together cannot explain all that we have seen so far in the blue whirl.
– How is the blue whirl related to standard swirl combustion?

  It is, in fact, more to whirl combustion [5], as the inflow is tangential rather than axial. A major point is that both whirl and swirl combustion are turbulent and rely on turbulence for mixing and reaction. The blue whirl is laminar. The blue structure in both whirl and swirl combustion have very different shapes than the blue whirl. Finally, both of these types of combustors are primarily used for gaseous, usually lean fuels. To date, the blue whirl relies on self-regulating evaporation of liquid hydrocarbons.

Background on Project Goals and Deliverables

The General Physical and Numerical Problem

There were three major deliverables outlined for this proposal. Here we give some background to explain why these are necessary precursors to building a simulation of a blue whirl.

An unsteady numerical simulation of a chemically reacting flow, such as a fire whirl or the blue whirl, consists of a series of submodels that describe the relevant physical properties and then models for connecting the results of the various submodels. The underlying framework is a model for the fluid dynamics, which is usually based on the Navier-Stokes equations (NSE). To this set of equations, various terms (submodels) are added that describe physical processes not fundamentally included in the convection of the fluid variables in the NSE. These include, for example, models describing how the chemical reactions, physical diffusion, and any other possible processes can alter the flow field, local energy and temperature, species profiles, etc. A set of boundary and initial conditions are needed to close the NSE. Each of these added processes has its own particular issues that have to be addressed. (Much of the this and the details of implementation have been discussed in [6].

Consider first the NSE, which describes the primary fluid variables, $(\rho, \rho\mathbf{v}, E)$, the total density, momentum, and energy, respectively. All of these are functions of position and time, $(\mathbf{x}, t)$. These variables are described by the set of equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, \mathbf{v}) = 0 \ , \tag{1}$$

$$\frac{\partial (\rho\, \mathbf{v})}{\partial t} + \nabla \cdot (\rho\, \mathbf{v}\mathbf{v}) + \nabla P + \nabla \cdot \widehat{\boldsymbol{\tau}} = 0 \ , \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + P)\mathbf{U}) + \nabla \cdot (\mathbf{v} \cdot \widehat{\boldsymbol{\tau}}) + \nabla \cdot (K\, \nabla T) = 0 \ , \tag{3}$$

where ρ is the mass density, $\mathbf{v}$ is the velocity, E is the energy density, P is the pressure, K is the thermal conduction coefficient, and

$$\widehat{\boldsymbol{\tau}} = \rho\nu \left(\frac{2}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} - (\nabla \mathbf{v}) - (\nabla \mathbf{v})^{\dagger} \right) \tag{4}$$

is the viscous stress tensor which includes terms arising in compressible Navier-Stokes equations with zero bulk viscosity. Here ν is the kinematic shear viscosity, $\mathbf{I}$ is a unit matrix, and superscript $\dagger$ indicates matrix transposition. Assume now that the equation of state required to close the NSE, a relation connecting pressure and density, is that of an ideal gas, so that

$$P = \frac{\rho R T}{M} \ , \qquad \epsilon = \frac{P}{(\gamma - 1)} \ , \tag{5}$$

where $\epsilon = E - \rho\, v^2/2$ is the internal energy density, γ is the adiabatic index, R is the universal gas constant, and M is the molecular weight.

Besides basic fluid flow changing the distribution of the primary variables, there can also be chemical reactions among the constituent molecules. Such reactions change the values of the primary variables through *local* changes in the chemical composition and energy deposition in the system. Other source terms that might be added to the NSE, in addition to chemical reactions, are physical diffusion terms, such as mass, heat, and radiation transport, and sometimes an additional set of equations representing multiphase processes, such as soot formation or particulate interactions. Each of these involves its own specific input parameters and issues related to the numerical implementation. The result of these additional physical or chemical processes can be included as source terms in the NSE. Here, however, for this first-pass simulation of a fire whirl and blue whirl, we begin by including submodels for heat and mass transport, chemical reactions and heat release, and by ignoring possible radiation transport. Omitted processes can be considered at a later time as needed.

With this background, we now address the issues of how to solve this set of equations, which leads to an explanation of the reason that code development was needed for fire whirls and the blue whirl.

The Fluid Dynamics Problem: The Flow Regime

In general, the set of NSE given above is solved very differently depending on the flow regime of interest. The differences are in both the approximations and numerical implementations of these approximations. Here we use a finite-volume approach, where space and time are divided into finite, contiguous elements. We solve the NSE for the behavior of the fluid as as function of time as it moves through these elements.

When the flow Mach number is high, that is, the fluid velocities approach or exceed the speed of sound in the fluid, sound waves are an important part of the solution. The methods used to solve problems in this regime are called "explicit" methods. These are the most straightforward, reliable, robust approaches to solving any set of coupled conservations equations, such as the NSE. The cost, however, can be high because the numerical time step used to evolve the solution is based on the reciprocal of the sound speed, and so it is very small. (As an aside, the presence of stiff chemical reactions can reduce this time step even further.) For our 3D, reacting flow problem, it might be possible to use the world's largest supercomputer to solve the equations this way, but it would still mean a very limited number of solutions and limited exploration of the regimes and dynamics of the reactive flow. We need something *very much faster*.

The other extreme is to remove *all* of the sound waves and assume incompressible flow, which means that sound waves travel at infinite speed and there is instant equilibration in the flow. Here, in principle, you could take larger computational time steps, perhaps based on the fluid velocity or another limiting processes (such as, e.g., diffusion). Methods for incompressible flow, however, are often unstable for three-dimensional unsteady flow with combinations of open and closed boundaries. In fact, acoustic waves *are* important in all combustion flows, and their presence helps stabilize the computation.

Thus the ideal approach might be to leave some of the sound spectrum in the simulation, perhaps enough to stabilize the flow, but allow us to go beyond the strict limit imposed by acoustic waves. This is the approach developed in this STIR program and described in more detail in the results section below.

The Chemical-Reactions Problem: Reducing Large Chemical Mechanisms

Chemical reactions and subsequent energy changes are usually computed by solving a set of ordinary differential equations (ODEs) representing reactions among the constituent chemical species. In the past years, this has led to chemical kinetic mechanisms for combustion reactions that have grown in size and complexity as more and more possible species and reactions are included. For example, a reaction mechanism for hydrogen-air could contain 50 chemical reactions among 9 species. For heptane-air however, it could contain over 500 species whose interactions are described by over 2500 reaction rates [7]. In principle, these models could be incorporated as source terms in the NSE, so that the evolution of the chemical reactions and heat changes are computed at each computational time step. The result could be an unreasonably expensive computation for a 3D unsteady flow.

Because of this expense, many methods have been developed to reduce the chemical mechanisms to a more manageable size. For example, one reduction of the large heptane-air [7] mechanism has only about 200 species interacting through about 800 chemical reactions [8]. Some of the approaches to constructing reduced mechanisms are reviewed in [9, 10].

The chemical-diffusive model (CDM) is an approach developed to replace the usual way chemical kinetics is incorporated in a fluid computation. The large set of ODEs representing both chemical reactions is now replaced by a mathematical expression describing conversion of fuel to product. (Physical diffusion processes are treated with the chemical reactions and similarly.) The expression contains a number of constants that are optimized to ensure that the results will, at least, give the correct combustion properties, such as the steady-state laminar flame speed and thickness, the adiabatic flame temperature, and 1D and 2D steady detonation properties. This approach, that is, using a submodel for chemical reactions combined with diffusion, has been used and continually refined and developed over twenty years now. It has been shown to produce surprisingly accurate predictions of flame acceleration and transition to detonation (e.g., [11, 12, 13]). More recently, an optimization procedure for finding the parameters was outlined and tested [14]. The CDM does, however, use the full chemical reaction models and any other available theoretical and experimental data available to optimize its input parameters.

When the CDM is used, the NSE including the chemical source terms become:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, \mathbf{v}) = 0 \ , \tag{6}$$

$$\frac{\partial(\rho\,\mathbf{v})}{\partial t} + \nabla\cdot(\rho\,\mathbf{v}\mathbf{v}) + \nabla P + \nabla\cdot\widehat{\boldsymbol{\tau}} = 0\ , \tag{7}$$

$$\frac{\partial E}{\partial t} + \nabla\cdot((E+P)\mathbf{v}) + \nabla\cdot(\mathbf{v}\cdot\widehat{\boldsymbol{\tau}}) + \nabla\cdot(K\,\nabla T) + \rho\,q\,\dot{\omega} = 0\ , \tag{8}$$

$$\frac{\partial(\rho\,Y)}{\partial t} + \nabla\cdot(\rho\,Y\mathbf{v}) + \nabla\cdot(\rho D\,\nabla Y) - \rho\,\dot{w} = 0\ , \tag{9}$$

where Y is the mass fraction of a reactant, $\dot{w} = dY/dt$ is the reaction rate, q is the total chemical energy release, and D is the mass diffusion coefficient.

We use the Arrhenius form for the conversion process:

$$\frac{dY}{dt} \equiv \dot{w} = -A\rho\,Y e^{-E_a/RT}\ , \tag{10}$$

where A is the pre-exponential factor, and E_a is the activation energy. The reaction rate $\dot{w}$ is proportional to ρ to account for the binary nature of chemical reactions taking place in typical combustion systems.

We assume that kinematic viscosity, diffusion, and heat conduction have a similar temperature dependence,

$$\nu = \nu_0\frac{T^n}{\rho}\ ,\quad D = D_0\frac{T^n}{\rho}\ ,\quad \frac{K}{\rho C_p} = \kappa_0\frac{T^n}{\rho}\ , \tag{11}$$

where ν_0, D_0, and κ_0 are constants, $C_p = \gamma R/M(\gamma-1)$ is the specific heat at constant pressure, and $n = 0.7$ emulates a typical temperature dependence of these coefficients in reactive hydrocarbon systems.

Recent work performed for the Alpha Foundation for the Improvement of Mine Safety and Health, Inc. required computations of flame acceleration in homogeneous and inhomogeneous methane-air mixtures. For that project, the CDM was generalized to be able to account for variable stoichiometry [15], so that it would be possible to compute flame acceleration in background reactive gases containing gradients in equivalence ratio. This led to the *possibility* that the variable stoichiometry CDM could be used to compute the properties of diffusion flames. The initial tests of this concept were carried out in this STIR program and will be described below.

Other Possible Effects: Soot and Radiation Transport

Just as it is necessary to use a reduced chemical model in a way that is fast and gives qualitatively correct results, it is also necessary to treat soot formation and radiation transport in a similar manner. For example, it is possible to use a two-equation soot formation model (e.g., [16]) that includes terms for soot nucleation, agglomeration, surface growth and oxidation. For radiation transport, it should be possible to use, for example, the Variable Eddington model (VEM) [6]. Incorporating these processes, while possibly important, were not covered in the initial development of the fire whirl model done for this proposal and left for future work.

Tasks of this Proposal

There were three main tasks in this proposal:

1. Fluid Dynamics: Test the basic fluid algorithm for solving the unsteady, compressible Navier-Stokes equations by predicting vortex breakdown in the same general regime of temperature and pressure as the blue whirl.
2. Chemical Reactions and Flames: Develop a calibrated CDM model for heptane-air vapor combustion. The model should cover a range of equivalence ratios from fuel-lean to fuel-rich conditions.
3. Fire-Whirl Simulation: Produce a first-pass simulation for conditions that might evolve into a blue whirl. Coordinate this with ongoing experiments at ARL Adelphi and UMD.

Results of Task 1: The Fluid Dynamics Solution

Our initial approach to simulating a fire whirl was essentially the same as the brute-force approach carried out previously [17]. Those prior simulations solved the full set of compressible 3D Navier-Stokes equations using the Flux Corrected Transport (FCT) algorithm (see, e.g., the recent review [18]) with a model for energy release into a vortical flow. More specifically, the equations were solved using an explicit (that is, the computational time step is small enough to resolve acoustic waves), high-order (fourth-order) monotone (no numerically generated unphysical maxima or minima are produced) method on a uniform, stationary Cartesian grid that was stretched at the boundaries.* These simulations were extremely expensive, in terms of both the required computer time and data storage. Only a rather limited range of the turbulence spectrum could be resolved. Nonetheless, the simulations were able to reproduce and evaluate the range of validity of a theoretically derived scaling law for fire whirls forming as a wind crosses an L-shaped object [17].

The current work in simulating fire whirls initially followed this same approach: We used a fully compressible version of FCT with an adaptive mesh that allowed local variations in resolution. For fire-whirl simulations, however, we fixed the grid in space and incorporated smoother transitions to a coarse grid towards the outflow. Again, the core region of the flame remained well resolved. Again, because the method was explicit, the cost of computing a 3D fire whirl for seconds or minutes of physical time was truly prohibitive. Very soon in the program it became obvious that we needed another approach.

Early in the development of reactive-flow algorithms, in particular, those specifically for low-velocity flame simulations, we proposed, developed, and tested a low-Mach-number method, BIC-FCT (Barely Implicit Correction to FCT) [19]. This allowed computations of premixed flames (e.g., [20, 21]) and axisymmetric diffusion flames (e.g., [22, 23]). This algorithm [19] changes the explicit solution to one that is "implicit," so that for low-velocity flows, the time step required is based on the fluid velocity and not on the acoustic speed. This first version of BIC was, however, difficult to use. In particular, it was hard to implement stable, nonreflecting boundary conditions at outflows. Optimization and controller algorithms along with filters were required to damp unwanted reflections, and these had to be modified on a case-by-case basis.

* FCT was the first method derived that could produce accurate solutions of the continuity equations and coupled continuity equations without introducing artificial diffusion added at discontinuities. The history of this development is reviewed in [18] and its principles are given in [6].

The main new step in BIC was a pressure correction derived from the implicit form of the momentum and energy equations. This pressure correction is obtained by solving an elliptic equation, to incorporate pressure changes at each time step. More exactly, there was a predictor step for density and momentum with a large time step, here determined by the fluid velocity, and implicit solution of an intermediate energy, and then the evaluation of the change in pressure (δP) over the time step which is used to correct the variables. This approach works well enough for the original test problems and for the Euler equations, but it did not work well for the full NSE, with or without additional source terms.

The new version of BIC-FCT, described in a paper recently submitted to *Computer and Fluids* [24], has several changes. First, there is now a source term in the energy equation that can be used to accumulate the effects of changes due to added source terms. In addition, it uses high-order monotone filtering steps to remove unphysical oscillations in the flow. This new approach was tested extensively. Results of test problems have been compared to fully explicit computations. Below we extract and describe two of the test problems from [24], one a simulation of a 2D doubly periodic shear layer, and the other a computation of vortex breakdown in a compressible flow.

Two-Dimensional Doubly Periodic Shear Layer

As a first example, consider a doubly periodic (2D) shear layer. The initial conditions for this problem are shown in Figure 2, which shows the computational domain on which a horizontal jet is initialized with small vertical perturbations. At the jet boundaries, the two shear layers roll up into large vortices as the flow evolves.

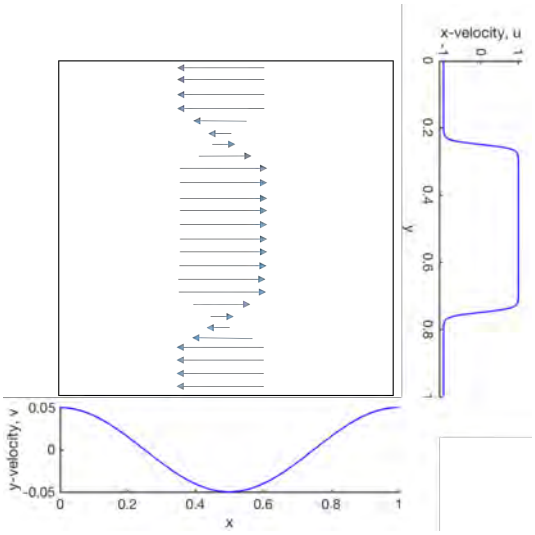

Figure 2. Initial velocity conditions for doubly periodic shear layers.

As [24] describes, the results of solving the NSE for this configuration were tested as a function of many parameters, both physical and computational. Perhaps the most important result for us now is related to the relative computational speed of the implicit and explicit solutions. Figure 3 shows a typical result for which both computations are done for 0.8 seconds of physical time. The results of the explicit and implicit solution are essentially indistinguishable, both qualitatively and quantitatively. Details of this are discussed in [24].

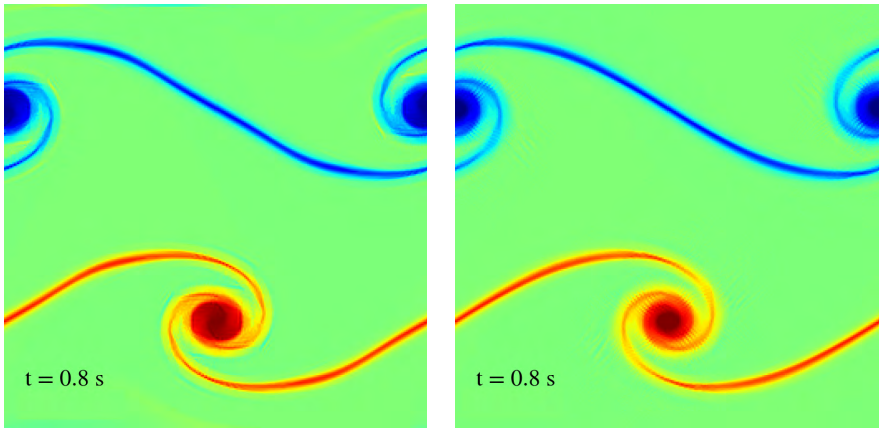

Figure 3. The doubly periodic shear layer computation on a 256×256 computational mesh. The BIC computation (right) is approximately 100 times faster than the explicit FCT computation (left).

Three-Dimensional Vortex Breakdown

We then began 3D tests of the new BIC algorithm by configuring the code to solve a the problem of 3D vortex breakdown in a compressible gas with both the explicit FCT and the implicit BIC-FCT. A computation of 3D vortex breakdown in a gas flow is a true test the ability of a calculation to predict the instabilities that occur in unstable swirling and whirling flows, such as fire whirls and swirl combustors. It is also a test that gives us some intuition about vortex breakdown in fire whirls, which could lead to a blue whirl.

The phenomenon of vortex breakdown results when a 3D axisymmetric vortex structure is affected by disturbances imposed by the combination of unsteady fluid dynamics, physical boundaries, or temperature. These disturbances can cause adverse pressure gradients near and on the spinning vortex core. When the axial momentum of the flow is not sufficient to overcome the force generated by the adverse pressure gradient, the vortex structure forms a new stable state. This state is characterized by a stagnation point on the central axis of the vortex with a recirculation zone around it. This change in the vortex structure is referred to as "vortex breakdown."

Based on distinctive structures that are formed, vortex breakdown was characterized into three types [25]: the spiral mode, the bubble mode, and the double-helix mode. All together, seven modes were reported [26], which include more intermediate states. Extensive research has been done over the past on this phenomenon as it appears in liquids in channels. This led to the conclusion that the types of breakdown are mainly controlled by the flow Reynolds number and the swirling level. Here, we adopt a set of flow parameters (swirl and Re) from a prior simulation [27], but now we are simulating a compressible gas flow. Under this selected flow condition, the vortex undergoes three major types of breakdown.

In the calculations we performed, the flow was initialized with a "Grabowski vortex" profile (also adopted by [27], originally introduced by [28]). This initialization is shown in Figure 4. The azimuthal, radial, and axial velocities vary with the radial location r, and the swirl number is defined as $S = v_\theta(R)/v_{z,\infty}$, where R is the radius of the vortex core, and the Reynolds number is $Re = v_{z,\infty}R/\nu$. The coflow parameter, $\alpha = v_{z,c}/v_{z,\infty}$, describes an axial velocity as a jet-like

($\alpha > 1.0$) or wake-like ($\alpha < 1.0$) profile. Here we have set $Re = 300$, $S = 1.3$, $\alpha = 1$, $R = 1$, and $v_{z,\infty} = 1$ m/s. The initial pressure and azimuthal velocity profiles are shown in 4. The simulations are performed on a 40 m $\times$ 40 m $\times$ 20 m domain in which the z-axis is the axial direction.

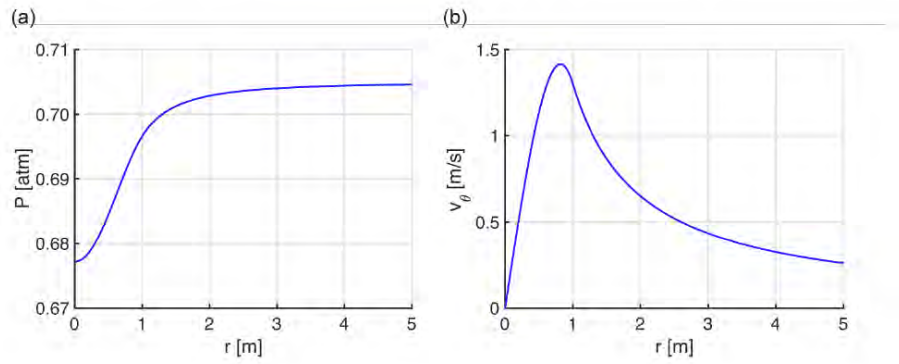

Figure 4. Grabowski vortex profile with swirl number $S = 1.3$, $\alpha = 1$. (a) Pressure distribution; (b) Azimuthal distribution.

Figure 5 shows two figures, which are frames extracted from movies of the computational results, the upper result from an explicit FCT computation and the lower result for a BIC computation. The flow has evolved from an unperturbed flow until a physical time of almost 3 minutes, using the different algorithms. The flow is going from left to right.

The flow is visualized by releasing massless particles at the inflow and allowing streaklines to carry them into the flow. The particles are superimposed on a background of normalized pressure. The darker region in the background indicates higher pressure and the lighter region indicates lower pressure. (The exact pressure normalization is as part of the figure.) The particles are released from 18 locations distributed evenly along a circle centered at the vortex axis with a 5 cm radius. The particles released on the circle are colored as black, white and grey, which here help to visualize the swirling motion represent different initial locations. At the center of the vortex, the particles are colored pink. Because the major portion of the vortex structure is at the center of the computational domain, only a small central section of the domain of 4 m $\times$ 20 m is shown in the figures.

An important point to make is that the BIC-FCT calculation was 20-30 times faster than the FCT calculation to obtain essentially the same physical time and results. To our knowledge, this is the first time that such an extensive full 3D flow computations have been compared for explicit and low-Mach-number solutions. The important result is that the simulation shows vortex breakdown and evolution to several of the nonlinear modes for a gas flow. In addition, as shown in [24], when the normalized results are compared to other computations, they are "right on."

As mentioned above, the ability to compute vortex breakdown and the evolution of the nonlinear modes is an extremely important part of the ability we will need to have to compute the evolution of a fire whirl to a blue whirl.

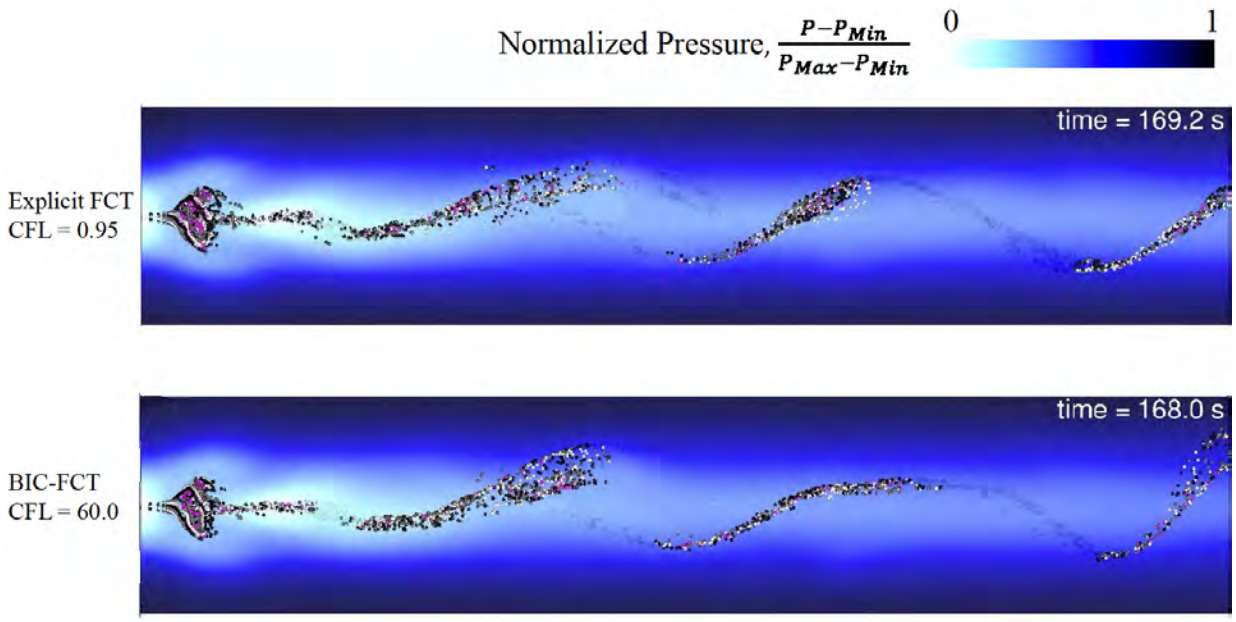

Figure 5. Frames extracted from movies generated from 3D unsteady computations of vortex breakdown for a system with Re = 300, Swirl = 1 on a computational grid of $40 \times 40 \times 20$ m^3. Only a portion of the computational domain is shown in the figure. Frames show normalized pressure. The top frame is from the explicit FCT computation and the lower frame is from the implicit BIC computation. The BIC computation is approximately 25 times faster. The video of these calculations can be found https://youtu.be/6qe7Mj2Iyuc

Results of Task 2: The Chemical Model

The fundamental idea of the CDM is to obtain values of the reaction parameters $\{\gamma, A, E_a, q, M\}$ and the diffusion coefficients, $\{\nu_0, D, \kappa_0\}$ which, when used in the NSE, reproduce correct, known physical properties of the reactive gas system. In the most general case, when we want to construct a chemical model valid for the full range of flow from laminar flames to detonations, we find the very best available values of flame and detonation properties (e.g., laminar flame speed S_l, adiabatic flame temperature, T_b, laminar flame thickness, Δx_L, Chapman-Jouguet detonation velocity, D_{CJ}, half-reaction thickness, x_d,) obtained from available full chemical models and experimental data, and use them in an optimization procedure to find the set of reaction parameters that reproduces these flame and detonation properties. This has been done for hydrogen-air, methane-air, and other energetic gases [11, 12, 13, 14]. In this way, we ensure that the energy deposition into the fluid system and conversion of fuel to product is correct, at least in the limits of laminar flames and detonations.

For the problem at hand, we are interested in simulating the behavior of heptane flames over a range of stoichiometries. Consequently, we concentrated on finding optimized parameters for flames and bypassed the detonation optimization. For this problem, we found the reaction parameters $\{A, E_a, q\}$ that reproduced the flame properties $\{T_b, S_l, \Delta x_L, \kappa_0\}$. Figure 6 shows the values of these flame properties obtained from the Cantera code [29] with a reaction mechanism consisting of 200 species and 800 reactions rates [8].

Now using the results of the CDM for heptane shown in the above figures, the NSE can be solved for a variety of flame problems. Figure 8 shows a calculation of a 1D laminar flame in a homogeneous stoichiometric heptane mixture using the new CDM parameters, and compares results from the implicit BIC and the explicit FCT algorithms. For this figure, the spatial x coordinate is centered at max(abs(dT/dx)). The computational cell size is 0.05 mm. The results are almost exactly the same, but the BIC time to calculation was faster by a factor of approximately 30.

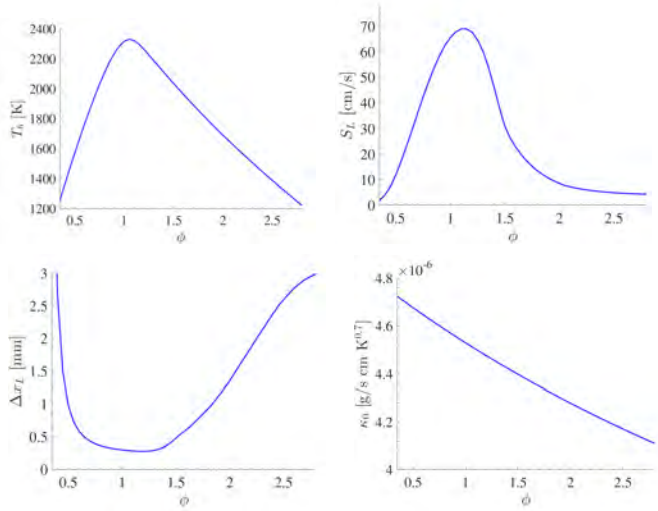

Figure 6. Adiabatic flame temperature, laminar flame speed, laminar flame thickness, and thermal conductivity coefficient, as a function of equivalence ratio, obtained from Cantera [29].

From these input values and basic flame theory, we are able to find the values of $\{A, E_a, q\}$ shown in Figure 7 to use as input chemical and diffusion model parameters directly in the NSE. Note that K is found from κ_o.

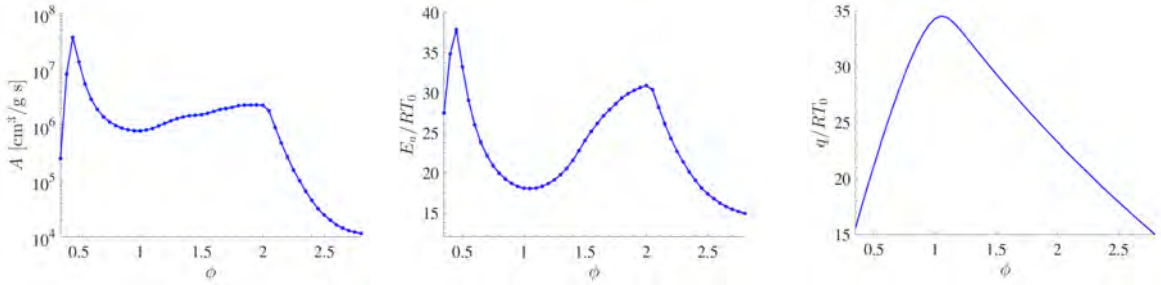

Figure 7. Optimal reaction parameters, A, E_a and q, obtained from the CDM, that reproduce the flame properties shown in Figure 6.

Now using the results of the CDM for heptane shown in the above figures, the NSE can be solved for a variety of flame problems. Figure 8 shows a calculation of a 1D laminar flame in a homogeneous stoichiometric heptane mixture using the new CDM parameters, and compares results from the implicit BIC and the explicit FCT algorithms. For this figure, the spatial x coordinate is centered at max(abs(dT/dx)). The computational cell size is 0.05 mm. The results are almost exactly the same, but the BIC time to calculation was faster by a factor of approximately 30.

The final tests of the chemical model would be whether it could compute a diffusion flame. For any problem in which the stoichiometry varies through the simulation, the set of reactive NSE given above must be modified to keep track of the changing proportionality of the fuel to oxidizer as a function of time and position. To this end, additional variables must be convected to ensure that the correct account of material is converted to release the correct amount of energy into the system. There are several ways to do this, but the current approach is to carry additional conservation equations for three species: fuel, oxidizer, and product. Then we compute a progress variable using those three species. A model for interspecies diffusion is included.

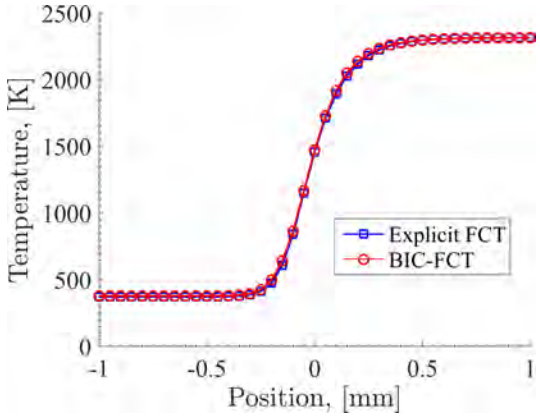

Figure 8. A 1-D laminar flame profile, using the CDM reaction parameters for a stoichiometric heptane-air mixture, for calculations using explicit FCT and BIC-FCT.

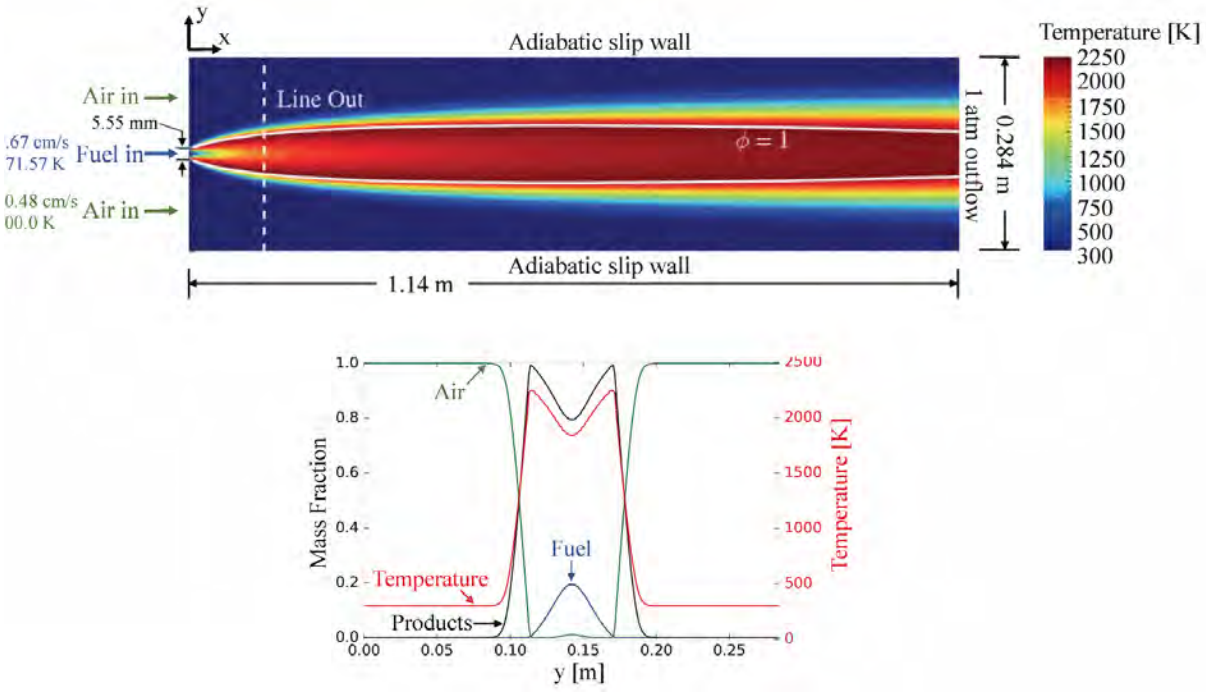

Figure 9. Laminar diffusion flame computed with heptane CDM and BIC-FCT.

Figure 9 contains a description of the test 2D diffusion flame problem underway now. For a problem such as this, considerable resolution is required in the diffusion regime. Exactly how much is required is being calibrated now and is work in progress. A comparison to experiments, either for this case or perhaps for a methane-air flame would help us to determine how well we must optimize the model for the diffusion parameters.

Results of Task 3: A Fire Whirl

This is the ultimate test problem: Can we compute a realistic fire whirl that burns heptane? In fact, this itself is a research problem in progress, and the first step towards a simulation of a blue whirl. It combines the algorithms and submodels we have developed to date: the new BIC algorithm and the variable-stoichiometry and diffusion flame models for heptane and air. It requires resolution of enough levels of turbulence.

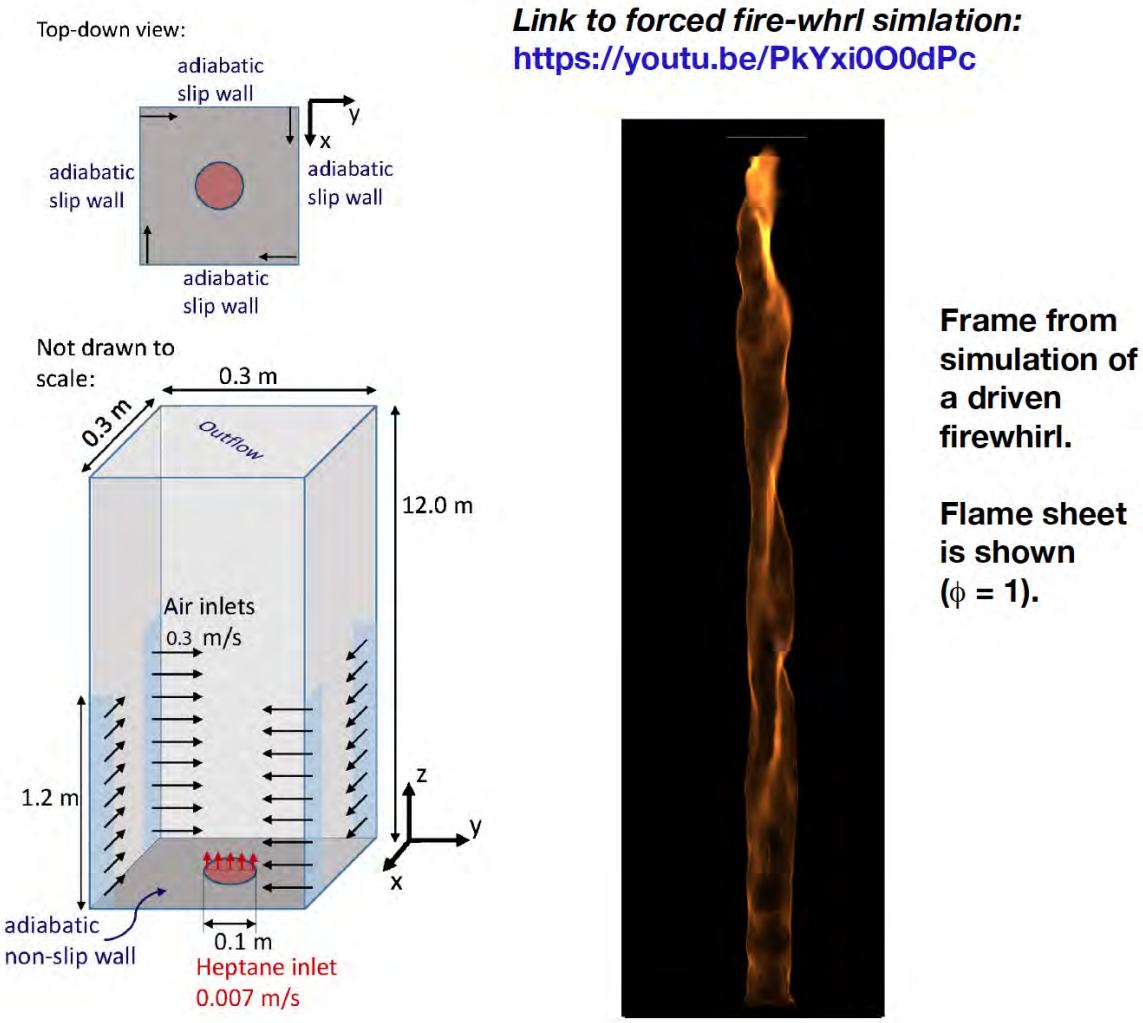

Figure 10. The CDM and 3D BIC-FCT combined to simulate a forced fire whirl. Left top: schematic viewed from top down. Left bottom: schematic of the computational domain. Right: Frame from a simulation of a driven fire whirl. Yellow color indicates the flame surface (stoichiometry = 1.0).

Figure 10 summarizes the results to date and gives a reference for seeing the simulation. The upper left figure shows the inflow conditions. The lower left figure is a 3D schematic of the problem. Here air is injected into a square container from four vertical holes at the bottom corner. Heptane fuel enters from a hole at the bottom.The total system is 12 m high, and the first 1.2 m allow air inflow. The outflow boundary is at the top. The frame on the right is taken from the simulation. The yellow regions indicates the $\phi = 1$ contour. This fire whirl is driven by the inflow, which creates a vortex and entrains the entering heptane vapor.

Summary and Conclusion: Future Directions

At this point, most of the tools we need to simulate a blue whirl and a fire whirl have been developed. They are not, however, completely tested and there are questions to answer. Any continued research in this area must:

1. Complete the testing of the CDM for diffusion flames and determine if the diffusion parameters must be improved. This will involve testing against any available data. Most likely, tests will be made for methane-air diffusion flames, as considerable experimental data is readily available. In addition, more calibration of the resolution needed in the diffusion region is required.
2. Continue computations of the heptane fire whirl. Then using what we have learned to create stable, optimized fire whirls, we need to analyze them for generic flow features and compare these, to the extent possible, to theory and experiments.
3. Configure the simulation to try to reproduce the conditions of vortex breakdown and to a blue whirl observed in experiments. This will involve either allowing the air inflow velocity to create the level of circulation seen in a fire whirl, or driving it to the circulation measured. In any event, the simulation has to be brought into the blue whirl regimes of circulation and energy release in which the blue whirl is observed.
4. Complete papers planned for this project. The paper
   * The paper *The Barely Implicit Correction Algorithm for Low-Mach-Number Flows*, Zhang, Chung, Kaplan and Oran, is under revision now for *Computers and Fluids*.

   Other papers that will be given at the 2019 AIAA SciTech meeting are:
   * *Vortex Breakdown in Gas Flows: A Comparison of Implicit and Explicit Simulations*, X. Zhang, J.D. Chung, C.R. Kaplan, and E.S. Oran
   * *Low-Mach-Number Simulation of Diffusion Flames with the Chemical-Diffusive Model*, J.D. Chung, X. Zhang, C.R. Kaplan, and E.S. Oran

   Other short abstracts and presentations will be submitted to the meeting of the American Physical Society Division Fluid Dynamics for presentation in November 2019.

Finally, all of the models and algorithms developed for this program do, in fact, go way beyond use for the blue whirl. These are generic and can be used for simulation of many types of high- and low-speed chemically reacting flows.

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