

Flame Acceleration Distance in Obstacle-Laden Tubes

Anke Vesper, Wolfgang Breitung, Sergey Dorofeev
 Institut für Kern- und Energietechnik
 Forschungszentrum Karlsruhe
 Postfach 3640, D-76021 Karlsruhe, Germany
 veser@iket.fzk.de, breitung@iket.fzk.de, dorofeev@iket.fzk.de

Alexander Efimenko
 Russian Research Centre Kurchatov Institute
 Kurchatov Sq. 1, 123182 Moscow, Russia
 efimenko@iacph.kiae.ru

Extended Abstract

Numerous experimental data on combustion of gaseous mixtures in obstacle-laden channels show that three characteristic combustion regimes can be distinguished in this type of geometry. These regimes include slow subsonic deflagrations, fast deflagrations, and quasi-detonations. Generally, cases of fast deflagrations and detonations can result in significantly high values of overpressures, which can be dangerous for integrity of confining structures. Considering practical applications for safety analyses, two important problems should be solved. The first one concerns the possibility of development of the fast combustion regimes in a particular mixture and geometry. If the fast deflagrations and quasi-detonations are principally possible, the second problem should be solved: evaluation of the minimum run-up distance for development of these fast combustion waves. While the first problem can be addressed with application of criteria for different combustion regimes (see, e. g., [1]), the second one should generally require application of a model for time-dependent simulation of the flame acceleration process.

The problem of the minimum run-up distance for the flame acceleration to supersonic combustion regimes in tubes with obstacles is studied in the present work both experimentally and numerically. Experiments were made in an explosion tube equipped with orifice plate obstacles. The tube was of 12-m long with internal tube diameter of 0.35 m. Blockage ratios (BR) of the orifice plates were 0.3, 0.45, 0.6 and 0.75. Hydrogen-air mixtures with 11 to 20 vol. % of hydrogen were used in the tests. The flame acceleration distance was defined from the dependence of the flame speed versus distance along the tube as a distance, where the flame speed reaches the value of 95% of the choked flame speed for each value of BR (close to the sound speed in combustion products).

The process of flame acceleration in a geometry, which is similar to the experimental one, was simulated numerically with 3D gasdynamic code B0B [2]. It was assumed that the effective turbulent burning rate is constant during all the process of the flame acceleration. This means that from two main factors responsible for the flame acceleration: increase of the flame surface due to interactions of gas flow with obstructions and increase of the burning rate with the increase of turbulence level, only the first one was accounted for in the simulations. The value of the effective turbulent burning rate was varied over a wide range representing maximum achievable turbulent burning rate for typical fuel-air mixtures, which is usually of the order of 10 times the laminar burning rate. The flame acceleration distance was defined in the simulations as a distance where the maximum local Mach number in the flow reaches unity. It was found that at this distance the flame acceleration is completed and a steady-state propagation of the flame follows the acceleration phase. It was found both in the tests and in the simulations that characteristic distance of the flame acceleration decreases with the increase of the blockage ratio and with the increase of the mixture reactivity (burning rate). It was found that the results of simulations reproduce correctly the flame acceleration distance found experimentally, if effective turbulent burning rate in calculations is chosen to be 10 times the laminar burning rate. This suggests that in the channel geometry with dense obstructions, with BR from 0.3 to 0.75, the geometrical factor (increase of the flame surface) is mainly responsible for the flame acceleration. On this basis a simple analytical model is suggested, which describes the evolution of the flame shape in the channel with obstacles. The dimensionless flame acceleration distance is determined in the model, which accounts for BR, laminar burning rate, and sound

speed in combustion products. The model allows to estimate the minimum acceleration distance necessary for development of the choked flames as function of mixture properties and geometrical parameters. The predictions of the model were found to be in a good agreement with experimental data obtained for a wide variety of mixtures in different tubes.

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Numerical Study of Combustion and Effects of Hydrocarbon Fuel Clouds

Georgy Makhviladze
Centre for Research in Fire and Explosion Studies
University of Central Lancashire
Preston PR1 2HE, UK
gmakhviladze@uclan.ac.uk

Sergey Yakush
Institute for Problems in Mechanics
Russian Academy of Sciences
Ave. Vernadskogo, 101
Moscow, 117526, Russia
yakush@ipmnet.ru

Extended Abstract

Accidental releases of flammable substances are a major hazard in the modern industry. Fuel-air mixtures formed in the atmosphere may explode or burn as large-scale diffusion flames known as fireballs. Uncontrolled combustion of large amounts of hydrocarbon fuels is dangerous because of powerful heat fluxes emitted during the fireball lifetime. While the integral characteristics of burning clouds (maximum diameter, burning time, emissive power) have been obtained experimentally, theoretical study of fireballs can provide further insight into the processes involved. In this work the fireballs from short-duration releases of hydrocarbon fuels into the atmosphere are modelled numerically.

The model for combustion of gaseous and pressure-liquefied hydrocarbons in the open atmosphere is based on the Favre-averaged Navier-Stokes equations closed by the $k - \varepsilon$ turbulence model and the eddy break-up model of turbulent combustion. Species transport equations are solved for O_2 , N_2 , CO_2 , H_2O and fuel vapour, temperature dependencies of thermodynamic properties of all components are taken into account. Soot formation is described by a two-step global kinetics submodel, while soot oxidation is assumed to be mixing-controlled.

The Weighted-Sum-of-Gray-Gases model is used to calculate the emissive properties of combustion products. Total of eight gray gases are used for the mixture of CO_2 , H_2O and soot. The radiative transfer equation for individual gray gases is solved using either the volumetric emission (no re-absorption) approximation or the P_1 -approximation depending on the optical thickness of fireball in the corresponding spectral group.

The dispersed phase is described on the basis of the Lagrangian approach with the random-walk model for turbulent diffusion. The droplets evaporate providing source of fuel for the gas-phase reactions.

Two main scenarios for the fuel cloud formation are studied. The first one is the short-duration vertical outflow of fuel from a pressurized vessel. In this case a transient fuel jet develops in the atmosphere during the release time, after which the vortex flow causes its transformation into a compact fuel cloud. Another type of event studied is rapid radial expansion of a volume of high-pressure gas or of pressure-liquefied fuel undergoing flash evaporation. This scenario is typical of bursts of pressure vessels (total loss of containment).

Calculations are performed for a wide range of initial conditions using methane, propane and butane as fuels. The internal structure of fireballs is revealed at different stages of evolution. For the vertical releases the burning jet transforms into a nearly spherical fireball shortly after the source terminates supply of the fuel. For the fuel clouds formed as a result of vessel burst the initial stage is featured by separation of the burning cloud from the surface, with its further transformation into a mushroom-like fireball.

Non-dimensional integral characteristics of burning clouds are introduced using the length, velocity and time scales which take into account gas expansion caused by combustion heat release. The scales are applicable to both single-phase and two-phase releases, as well as to the jet-like and instantaneous outflows. A unified description of the fireball non-dimensional lifetime as a function of the Froude number

(defined in terms of the ratio of initial release velocity and the characteristic velocity of buoyant flow) is given for each outflow scenario. The calculated results correlate well with the experimental data available.

Radiative characteristics of burning hydrocarbon clouds are determined for the fuel masses ranging from 1 g to 2000 kg. It is shown that fireballs become optically thick (so that their emissivity becomes as high as 0.8–1.0) for the fuel masses exceeding approximately 1 kg. The fraction of combustion energy emitted by the burning cloud as thermal radiation, is shown to be in the range 20–30%, which agrees with experimental observations for large-scale hydrocarbon flames.

The Monte-Carlo method is applied to calculate the radiative fluxes from the burning clouds incident on the ground surface. Also, thermal dosages are calculated by time integration of the fluxes. Differences between the distributions of fluxes and dosages obtained in the cases of vertical releases and instantaneous cloud formation are discussed.

Numerical Simulation of Fuel-Droplet-Propane Releases After Tank Failure

Sergei V. Utyuzhnikov

Department of Mechanical, Aerospace and Manufacturing Engineering
UMIST, PO Box 88, Manchester, M60 1QD, UK
s.utyuzhnikov@umist.ac.uk

Extended Abstract

The paper is devoted to a numerical simulation of fuel cloud behaviour following releases of a liquid fuel. The main aim of the work is to develop further a mathematical model to simulate such processes into the atmosphere. The model is validated by a comparison with experimental results. The influence of boundary conditions for turbulent kinetic energy k and ε its dissipation rate ε on the solution is investigated. It is concluded that the solution depends mainly on the combination of k and ε in the form $k^{3/2}/\varepsilon$ rather than each of these values separately. A way to define the boundary conditions for k and ε is suggested. The KIVA-II code has been used as the base of the code used. The original code has been modified to simulate low Mach number atmospheric flows, radiation, soot formation and turbulent combustion.

Many chemical industry accidents are accompanied by fuel releases. Usually, a large quantity of fuel is stored at high pressures in a liquid state. Even a small rupture can cause a quick release of fuel from a tank. A failure of a tank with pressurised fuel is followed by abrupt decrease of pressure, explosive boiling and evaporation two-phase outflows of a liquid-vapour-air mixture. An ignition of such a fuel-droplet-vapour-air cloud can cause shock-free combustion with the formation of a fireball. Powerful radiation flux, emitted by the fireball, is dangerous for people and the environment.

There are a number of papers devoted to numerical investigations of vapour fuel clouds combustion in the atmosphere. At the same time, combustion of two-phase releases of liquid fuel has not been studied well up to now. The present paper is a further development of the model presented in [1]. In a comparison with [1], the more comprehensive model for a droplet motion is used, a non-vertical fuel release is allowed. A special attention is paid to the boundary and initial values for turbulent variables.

The flow of a fuel-droplet-air mixture from a ruptured tank is considered. An Euler-Lagrange approach is used to solve the Navier-Stokes equations. The combustion process (the eddy break-up model), turbulence (the k - ε model) and radiation (the weighted-sum-of-gray-gases model) are taken into the consideration. Along with the radiation, soot formation is simulated. It is important because of the strong influence of soot on the radiant emittance of flame. The Lagrangian approach is used to simulate the dispersed droplets behaviour and describe the mass, momentum and energy exchange between the gas and liquid phase via the source terms. A one-phase gas model, where instantaneous evaporation of fuel liquid is assumed, is used along with the two-phase model. Numerical results are compared with the experimental results [2, 3].

The present investigations may be directly used in numerical simulation of the tank failure. The process of a tank failure is complicated because it is accompanied by destruction of the tank, fuel release under high pressure, intermixing of fuel and air, and combustion. Furthermore, these processes can take place simultaneously. It is very difficult or even impossible to describe all these processes in detail. Therefore, a simple model of the initial stage of the process is desirable. The main aim of this investigation is to develop such a model. A comparison with experimental data enables one to validate the model.

The k - ε model is used to simulate the turbulent processes. Inlet and initial boundary conditions for k and ε have to be specified. In this work, an approach was suggested to estimate the initial and inlet boundary conditions for k and ε . This approach is based on the results of our calculations which show that the mixing length Λ is a governing parameter to choose initial and boundary values for k and ε . It means that the solution depends more strongly on the inlet and boundary conditions for than Λ on the inlet and initial values of k and ε separately. The choice of inlet value of is Λ suggested.

The mathematical model developed was verified by a comparison with different experimental data [2, 3] concerned with the behaviour of releases, following tank failures with propane at high pressures.

The governing equations system for the soot formation is stiff. An effective numerical approach to integrate the system has been developed. The method is based on a local analytical solution that allows one to receive a positively defined scheme. The elliptical equations for the radiation problem are solved by the conjugate gradient method along with special preconditioning.

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Ignition and Flame Propagation in an Impulsively Started Fuel Jet

V. R. Katta*, T. R. Meyer*, J. R. Gord, and W. M. Roquemore

Propulsion Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, OH

Correspondence E-Mail Address: vrkatta@erinet.com

*Innovative Scientific Solutions, 2766 Indian Ripple Road, Dayton, OH.

Extended Abstract

It is possible to increase the burning velocity of the premixed gas by moving the flame into a region where fuel is traveling at a higher velocity. Studies by McCormack et al.¹ obtained flame speeds up to 15 m/s in vortices and suggested a linear dependence of flame speed on vortex circulation. Ishizuka et al.² also reported super-laminar flame speeds along the vortex core, but observed a somewhat reduced dependence on vortex circulation. Cattolica and Vosen³ performed studies of premixed flame propagation in the wake of a vortex for a combustion-torch configuration in which, ignition of lean premixed gases within a combustion chamber generated a vortex ring of unburned, premixed methane and air. The flame followed in the wake of the vortex eventually propagated through the vortex rollers. In the present paper a numerical investigation has been performed to understand the various flame propagation patterns that were observed in our experimental work on impulsively started jets and the vortices.⁴

Mathematical Model. The ignition and flame propagation was simulated using an unsteady two-dimensional code known as UNICORN.^{5,6} The time-dependent governing equations were expressed in cylindrical-coordinate system. Time and species dependent transport coefficients were employed. The detailed chemistry model employed for describing methane combustion consists of 17 species and 52 elementary reaction steps. The finite-difference forms of the momentum equations were obtained using an implicit QUICKEST scheme, and those of the species and energy equations were obtained using a hybrid scheme of upwind and central differencing. Computations were performed using a 571 X 151 non-uniform grid system covering a physical domain of 70 X 20 mm. The grid system was clustered to yield a local grid spacing of 0.1 mm in both the axial and radial directions. The burner diameter was 5 mm and a flat velocity of 0.135 m/s was used as initial flow condition. A fuel jet was issued into the flow by suddenly increasing the fuel velocity to 6.5 m/s. It consists of CH₄ and O₂ at stoichiometric proportions and 71.5% N₂. A steady annular air flow of 0.135 m/s was used throughout the calculation. Ignition was initiated at a location that is 2 mm above the inflow boundary and at the axis of symmetry. The delay between the start of the jet and the vortex (ignition-delay time, τ) was varied to investigate flame propagation through the injected premixed gases.

Results and discussion. A jet having a velocity of 6.6 m/s issued into a low-speed parallel flow generates a large mushroom-shaped vortex ahead of the jet. As the jet pushes into this nearly stagnant flow the size of the head vortex increases rapidly. Impulsively started jets also generate smaller vortices on the jet column just upstream of the larger vortex. As the head vortex convects downstream it entrains not only the surrounding air but also the secondary vortices on the jet itself. The jet tip is penetrating at a velocity of ~ 4.1 m/s.

Calculations were made for different ignition-delay times and the results for four different cases are shown in Fig. 1 in the form of temperature distributions and fuel-jet structures. These cases were selected to illustrate the different flame-propagation mechanisms. In Case 1, ignition was initiated 0.75 ms after the jet was started. By this time, the tip of the jet has traveled ~ 1 mm past the spark location and provided combustible mixture at the time of ignition. The flame and jet structures at 3.5 ms and 12.3 ms are shown in Fig. 1(a). The average velocity of the flame propagation in the axial direction is ~ 3.4 m/s, which is $\sim 17\%$ lower than the cold-jet propagation velocity. Flame in this case is established along the outer core of the fuel jet and is acting like a barrier to the fuel jet. On the other hand, as the laminar burning velocity of the stoichiometric methane-air mixture (0.38 m/s) is much less than the jet velocity, the flame is

propagating with the jet, but at a reduced velocity. This is the case even when the ignition delay was increased to 1.5 ms [Fig. 1(b)]. The average flame propagation velocity remained at 3.4 m/s as the flame wraps around the jet. However, there is a significant difference in the jet structure when it is compared with the one obtained for 0.75-ms ignition delay. Jet in the 1.5-ms case became transitional with the formation of ~ 420 -Hz organized structures, while the jet in the 0.75-ms case became laminar at $t = 12.3$ ms. Flame propagation completely changed when the ignition delay was increased to 6 ms [Fig. 1(c)]. Here, the head of the jet has traveled 24 mm past the ignition location by the time ignition was initiated. Flame has rapidly propagated downstream and caught up with the tip of the jet and the average burning velocity has reached a value 6.5 m/s. Since flame propagated into the head vortex from the wake region the former got expanded. Jet in this case also became transitional with the formation of organized structures. When the ignition delay was increased to 7 ms, flame tried to catch up with the jet tip but could not succeed [fig. 1(d)]. As a result, the initial fuel vortex formed at the tip of the jet got detached from the fuel jet and traveled as a pocket of unburned gas. The average burning velocity for this case has dropped back to 5.5 m/s.

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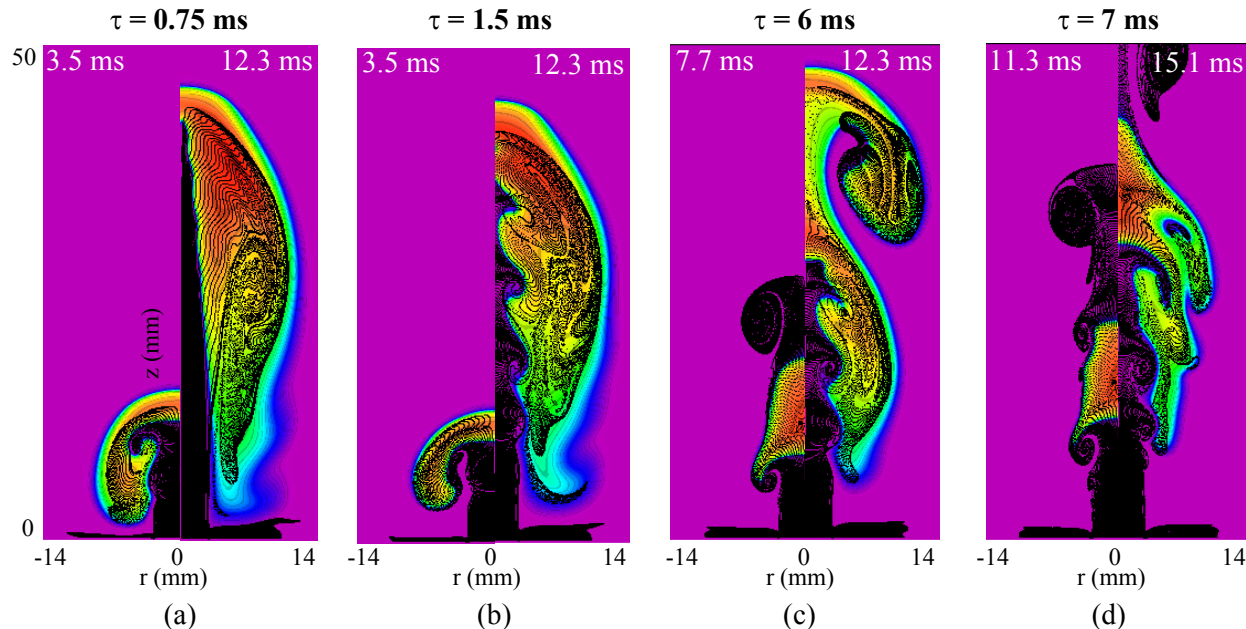


Fig. 1. Influence of ignition-delay time on flame propagation through a 5-mm-diameter fuel jet. Velocity of the jet is 6.5 m/s. In each picture locations of particles injected from fuel jet are superimposed on the temperature distribution. The ignition delays (a) 0.75 ms, (b) 1.5 ms, (c) 6.0 ms, and (d) 7.0 ms represent the time lapses between initiation of ignition and start of jet. Left- and right-half images represent flame structures during the early and later stages of flame propagation, respectively.

2D and 3D Simulation of Supersonic Hydrogen Jets Combustion in a Supersonic Air Flow

A. Kaltayev, A. Naimanova, Sh.A. Ershin, U.K. Zhabbaspayev
 Faculty of Mechanics and Mathematics
 al-Farabi Kazak National University
 Almaty, Kazakstan, kaltayev@yahoo.com

Extended Abstract

The research of gas-dynamic, acoustic, thermal and constructive conditions allowing to intensify a mixing of fuel jets with air-flow, plays the important role at creation of supersonic combustion of hydrogen in a scramjet combustor. Combustion characteristics at supersonic speed are defined by intensity of turbulent mixing processes, rate of chemical reactions in a flow and influence of gas-dynamic effects accompanying heat release.

The results of numerical simulation of hydrogen combustion in a supersonic air flow are given. The supersonic hydrogen jets ($T_2=254 K^0$, $M_1= 1.8$) injected into a supersonic air flow ($M_2=3.63$, $T_2=1270 K^0$, $n=1.1$, $Y_{O_2}^0=0.266$, $Y_{H_2O}^0=0.256$, $Y_{N_2}^0=0.478$) at different angles ($\alpha = 0; 30^0$).

The 2D and 3D turbulent mixing and combustion are governed by time averaged and parabolized Navier-Stokes equations using two-parametrical “k - l”- turbulent model and detailed kinetic mechanism of hydrogen oxidation:

$$\frac{\partial \vec{E}}{\partial x} + \frac{\partial (\vec{F} - \vec{F}_v)}{\partial y} + \frac{\partial (\vec{G} - \vec{G}_v)}{\partial z} = 0,$$

$$\vec{E} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E_t + p) u \end{pmatrix}, \quad \vec{F} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (E_t + p) v \end{pmatrix}, \quad \vec{G} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (E_t + p) w \end{pmatrix},$$

$$E_t = \rho h - p + 0.5 \rho \vec{v}^2,$$

$$p = \rho \frac{R}{W} T, \quad W^{-1} = \sum_{k=1}^K \frac{C_k}{W_k},$$

$$h = \sum_{k=1}^K C_k h_k(T), \quad h_k(T) = \int_{T_0}^T c_{p,k}(T) dT + h_k^0.$$

The kinetics of hydrogen combustion in the air is described by seven-stage mechanism and includes six components: H_2 , H_2O , OH , H , O :

$$\rho u \frac{\partial C_k}{\partial x} + \rho v \frac{\partial C_k}{\partial y} + \rho w \frac{\partial C_k}{\partial z} - \frac{\partial}{\partial y} (A \frac{\partial C_k}{\partial y}) - \frac{\partial}{\partial z} (B \frac{\partial C_k}{\partial z}) = \nu_k, \quad k = 1, 2, \dots, K,$$

The behavior of supersonic hydrogen combustion are considered and investigated in tasks:

- 1) A system of flat hydrogen supersonic jets is injected parallel and at different angles into a supersonic flow (Figure 1);
- 2) A system of round or elliptic hydrogen supersonic jets injected into a supersonic flow;
- 3) A system of round or elliptic hydrogen supersonic jets injected into a supersonic flow with subsonic zones.

The influence of fuel and oxidant parameters on completeness of hydrogen combustion was estimated.

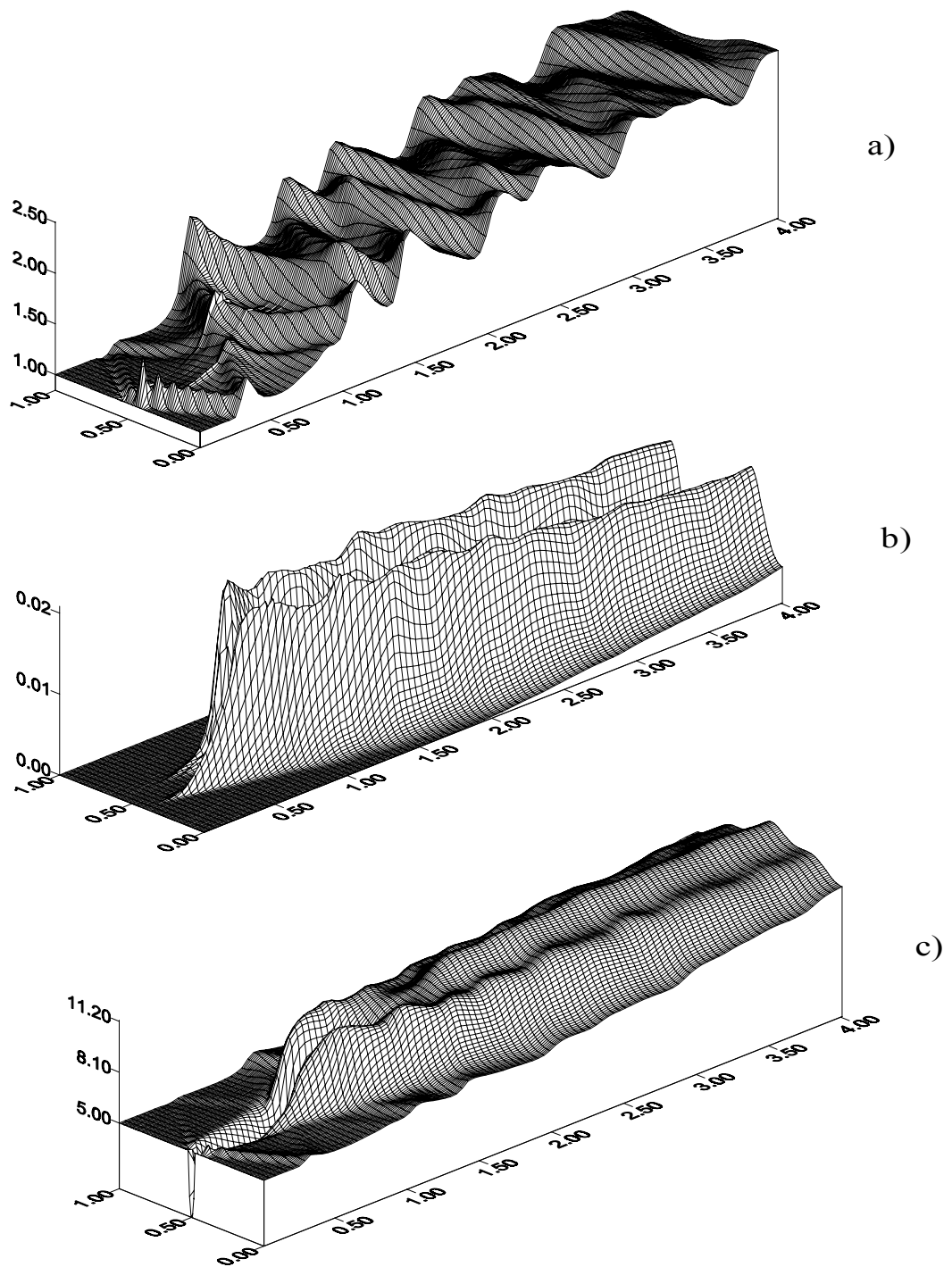


Figure 1. Pressure a), concentration OH b), and temperature c) fields,
 $M_1 = 1,8$; $M_2 = 3,6$; $T_1 = 254 \text{ K}^0$; $T_2 = 1270 \text{ K}^0$; $n = 1,1$; $\alpha = 30^0$;
 $Y_{O_2}^0 = 0,266$; $Y_{H_2O}^0 = 0,256$; $Y_{N_2}^0 = 0,478$.

Parallelization and Integration of a Large Scale Hydrocarbon Pool Fire in the Uintah PSE

Rajesh Rawat¹, Jennifer P. Spinti², Wing Yee³, Philip J. Smith⁴
University of Utah

Extended Abstract

Realistic simulation of complicated systems such as large-scale pool fires requires the representation of relevant physical processes such as turbulent reacting flows, convective and radiative heat transfer, and fundamental gas-phase chemistry. Moreover, such complex systems are characterized by a wide range of continuum length scales (1mm-1km) and corresponding time scales (1 fs-1 s).

Coupling these processes presents a unique challenge from both a research and a software engineering perspective. The entire range of length and time scales cannot be directly computed even on peta-flop computers, i.e., the next generation ASCI machines. Nevertheless, important features of fire physics can be captured by resolving the large length and time scales responsible for controlling the dynamic features of fire. Resolving these length and time scales, however, requires massively parallel computations. Therefore, we are developing software components that reuse physics-based legacy Fortran codes (Arches), are validated against experiments, and are computationally efficient and scalable. With these components, one can freely choose options for different turbulent flow models, turbulent mixing models, radiation models, and solvers and then couple them with the Uintah Computational Framework (UCF), a component-based, visual Problem Solving Environment (PSE) [1], to achieve parallel computations. The UCF provides the framework for the large-scale parallelization of different applications.

Integration Strategy

The integration of the legacy fire code in the UCF is built on three principles: 1) Develop different reusable, physics-based components that can be used interchangeably and can interact with other components, 2) reuse the legacy fire code (written in Fortran) as much as possible, and 3) use components developed by third parties, specifically non-linear and linear solvers designed for solving complex-flow problems.

Our first step was to design a generalized, component-based architecture for fire simulations that can be incorporated in any computational framework that provides support for parallelization. First, we worked on the software design specifications to integrate with the UCF. These components are designed around real world concepts (such as subgrid scale micromixing as represented by the MixingModel component), and they encapsulate functionality found in multiphysics problems. Many of the design decisions were necessitated by the parallel-processing paradigm provided by the UCF.

Parallelization Strategy

For parallel CFD computations, the UCF creates a task graph using the components provided by the application developer. It then assigns them to different processors determined by the Scheduler based on the cost model for computation and communication. Figure 1 shows a typical task graph created during the process of solving the pressure equation, one of the steps in a fire simulation.

¹ Department of Chemical and Fuels Engineering, rawat@crsim.utah.edu

² Department of Chemical and Fuels Engineering, spinti@crsim.utah.edu

³ Department of Chemical and Fuels Engineering, wing@crsim.utah.edu

⁴ Department of Chemical and Fuels Engineering, smith@crsim.utah.edu

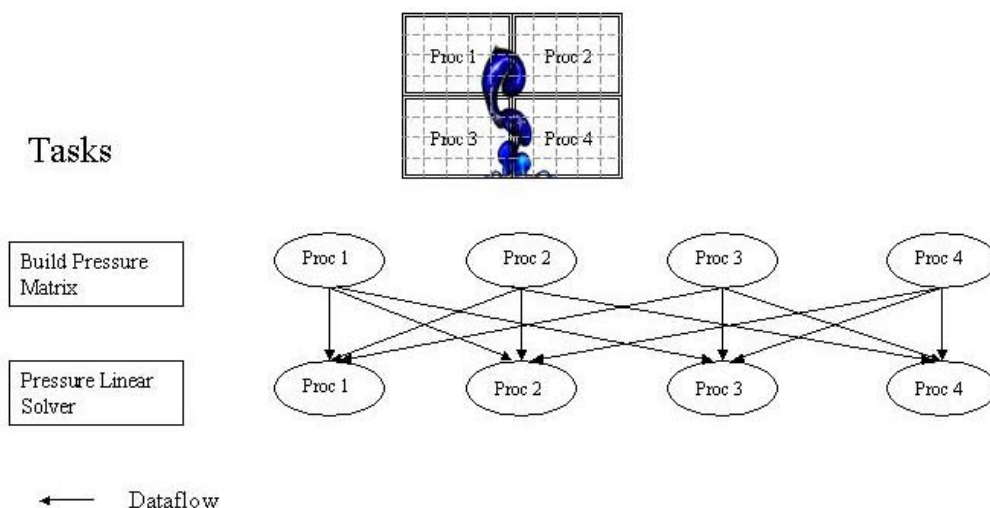


Figure 1: An example task graph for the pressure solver in Arches

This process has been divided into two tasks. In the first task, a linear matrix is generated through discretization and the application of boundary conditions. Before the start of this task, each processor has the data it requires for computing the matrix. In the second task, the matrix is solved using PETSc [2]. As shown in Figure 1, the computational domain is divided into four patches, and each patch is associated with a processor. Arrows in the figure indicate data dependencies between the processors. This task graph is used by UCF to determine dependencies and data transfer.

Results

The simulation of a 10-m heptane pool fire illustrates the parallel scalability obtained with the integrated UCF/Arches code. Linear scalability to 1000 processors is obtained on the SGI Origin 2000 at Los Alamos National Laboratory. To achieve scalability beyond 1000 processors, other preconditioners such as multigrid must be considered since the preconditioner used in this computation does not exhibit good scaling characteristics beyond 1000 processors.

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