# Vortices generation on the wall blowing surface with chemical reactions

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## I. Introduction

The stability and combustion behavior of unsteady motion in solid propellant rockets are significantly affected by two mechanisms. These are the generation of unsteady vortices at the burning surfaces and the coupling between acoustical motion and vortex shedding at obstacles or near the region adjacent to the burning surfaces. Despite of fundamental differences flow conditions at entrance of combustor; fully turbulent incoming flow in hybrid rockets and accumulated mass driven flow in solid motors, it is expected to observe a similar behavior of hydrodynamic instability in hybrid rocket associated with the interaction of vortex shedding. From the hydrodynamic point of view, flow dynamics in solid propellant rocket is very analogous to those in hybrid rocket in that flow instabilities are found as a consequence of coupling between mean flow and evaporative fuel flow from the surface. French research groups concentrated on the flow instability in solid propellant motor extensively.

The numerical studies with LES methodology by Na & Lee showed very interesting features of flow behavior near the wall surface. Their calculation results showed that the interaction of oxidizer turbulent flow with the wall injected flow can completely alter the structure of turbulent boundary layer and produce isolated cell-like contours of streamwise velocity near the surface.

Camicino et al. recently performed a series of combustion test with two different injector configurations; axial and radial types. They found that combustion behaviors were strongly dependent upon the interaction of vortex shedding and acoustic oscillations determined by injector configurations. However, more research is still required to understand the physics of the interaction of vortex shedding and acoustic oscillations. Thus, it is also quite interesting to ask what would happen if vortex shedding induced in the pre-chamber could interact with vortices formed as the result of instabilities with evaporative normal flow in the vicinity of burning surfaces.

Motivated by the question related to the flow conditions in hybrid rocket combustion, LES calculation with chemical reactions has conducted to find the behavior of hydrodynamic instability in the flow if vortex shedding from the pre-chamber interacts with vortices in the vicinity of burning surfaces as observed in solid motors.

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## II. Numerical Simulations

As depicted in Figure 1, the pipe consists of two regions: recycled part (-5<x/D< 0) and wall injecting part (0<x/D<10) where D is the diameter of the pipe. The recycled pipe is added to provide realistic turbulence without any discontinuity to the main region of interest. The wall injecting region is applied to simulate effect of a regression process of a hybrid rocket. The numbers of grid points used to discretize the computational domain in axial, radial, and azimuthal directions are 192, 64, and 128, respectively. In radial direction, meshes are gathered using hyperbolic tangent function to capture near-wall flow accurately.

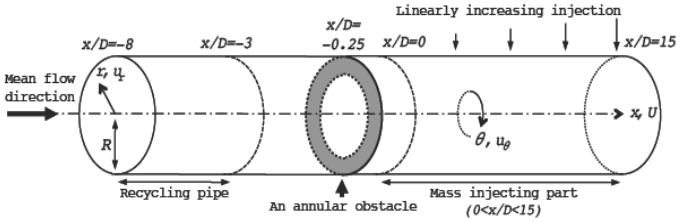


Fig 1. Computational domain for the case without and with a block

Secondly, a pipe with a ring-type block attached in front of wall blowing region is simulated. A schematic of this configuration is available in Figure 2. Lengths of the recycling and mass injecting parts are identical to the previous case. Length and height of the block is one-tenth of the diameter, from which vortex flow with substantial strength is generated. Then, interactions between the generated vortex and vortex shedding due to wall injection would occur.

Averaged axial velocity at inlet is 23.3m/s in this study, thus Mach number for substantial portion of the domain is very low. Therefore, a preconditioned compressible flow solver is used. A modified Roe-type flux difference scheme is used which is suitable for LES and viscous terms are calculated by central differencing. Time integration is done using a dual-time stepping method to allow larger time-step size. A dynamic Smagorinky sub-filter model is used to closure LES terms.

At the interface between recycling and injecting parts, all flow information is passed through except pressure since pressure-related wave is assumed to ravel backward. In this study, recycling (or recirculation) technique follows a method suggested by Leonard et al. While maintaining velocity and thermal fields at the same time is hard to achieve in a compressible flow, it was not a huge bottleneck for such low-speed flow.

### Chemical Reactions

To take reactions into account, the equilibrium combustion model is used [1]. The reversible chemical reaction is assumed to reach equilibrium state infinitely fast; thereby heat release of the final state can be directly exploited in the computation. Transport equation of a filtered conservative scalar is solved along with flow governing equations in LES. The conservative scalar is named as mixture fraction Z, defined as a following normalized formula when $Y_F$ and $Y_O$ are fuel and oxygen mass fractions and superscript 0 represents boundary values at fuel and oxidizer streams.

$$Z = \frac{\nu Y_F - Y_O + Y_O^0}{\nu Y_F^0 + Y_O^0}$$

For a $\nu_F'(\text{fuel}) + \nu_{O2}'O_2 \leftrightarrow (\text{product})$ reaction, stoichiometric oxygen-to-fuel mass ratio $\nu$ is defined as $\nu = \nu_{O2}' W_{O2} / \nu_F' W_F$. A transport equation for the filtered mixture fraction, $\tilde{Z}$, is,

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t} + \nabla \cdot \bar{\rho}\tilde{u}\tilde{Z} = \nabla \cdot \bar{\rho}\widetilde{D}\nabla\tilde{Z}$$

Mixture fraction is discretized into 100 sample values, which are properly clustered near stoichiometric point. For each mixture fraction value, CHEMKIN subroutine is used to calculate equilibrium state solution, which is saved on a file as a lookup table. Equilibrium calculation routine also offers enthalpy at the final state that can be used to calculate reaction source for the energy equation $\widetilde{s_h}$. However, to simplify the routine, heat source is calculated using temperature difference between that the equilibrium state and current temperature, or $\widetilde{s_h} = C_p(\widetilde{T_e(Z)} - \tilde{T})$ where $C_p$ is the heat capacity and $\widetilde{T_e(Z)}$ is the filtered temperature at the equilibrium state.

In LES, however, $\widetilde{T_e(Z)}$ is not identical to $T_e(\tilde{Z})$. A modeled subfilter probability density function $P(Z)$ is used to calculate filtered temperature for the equilibrium state for each computational cell [2].

$$\widetilde{T_e(Z)} = \int_0^1 T_e(\xi)P(\xi)d\xi$$

$P(Z)$ is assumed to follow a beta distribution that bases on the first two moments. The Smagorinsky-type subfilter variance model [3] is used to calculate second moment of the scalar while the first moment is directly obtained from the transport equation of $\tilde{Z}$. A lookup table is written in a separate file, which includes equilibrium temperature for 50 different variances for a given filtered mixture fraction. The combustion routine is integrated into the preconditioned compressible LES solver extensively used by the authors

**Results**

In the computation, a methane reaction is implemented. A methane-air reaction mechanism from GRI-Mech 3.0 is used [5]. The heat source, however, is reduced by half to avoid numerical instability. In fact, the solver used for current study does not have the shock capturing capability. Other computational details are identical to the without a block case in [4]. A cylindrical domain is discretized by 256, 64, and 128 cells in axial, radial, and azimuthal directions. A fully turbulent flow is generated through the periodic domain of $(-5 < x/D < 0)$, which is followed by the fuel injecting part $(0 < x/D < 15)$. Fuel is injected radially from the wall, with the linearly varying rate of 0% (at $x/D = 0$) to 3% (at $x/D = 15$) of the mainstream bulk velocity (23.3m/s). Reynolds number for the mainstream bulk velocity is 15,300.

Figure F1 shows reactive results from a plane view. Due to injected fuel, mass fraction is higher near wall and slowly penetrates toward the center of the pipe. Reaction appears highly active along where flow condition is in stoichiometric. However, flame appears not continuous in the contour as subfilter variance of the mixture fraction changes. Also the flame bands are detached from the wall due to high mixture fraction values near the wall. The high temperature band departs from the wall further as the flow goes downstream as in Figure F2. Thus, the reaction zone is close to the axis near the exit. Figure F3 shows temperature isocontour of 800K, which indeed comes toward the axis in the downstream. The isocontour is colored by slowly decreasing gas-phase pressure. Background is the axial velocity at $y^+ = 10$ location near wall, which shows lengthy velocity streaks.

Temperature for filtered mixture fraction of all computational cells of the result at one instant is given in Figure F4. While many cells follow equilibrium solution, some are deviated due to subfilter variance effect. Also, the deviation is partly due to the nature of convecting property.

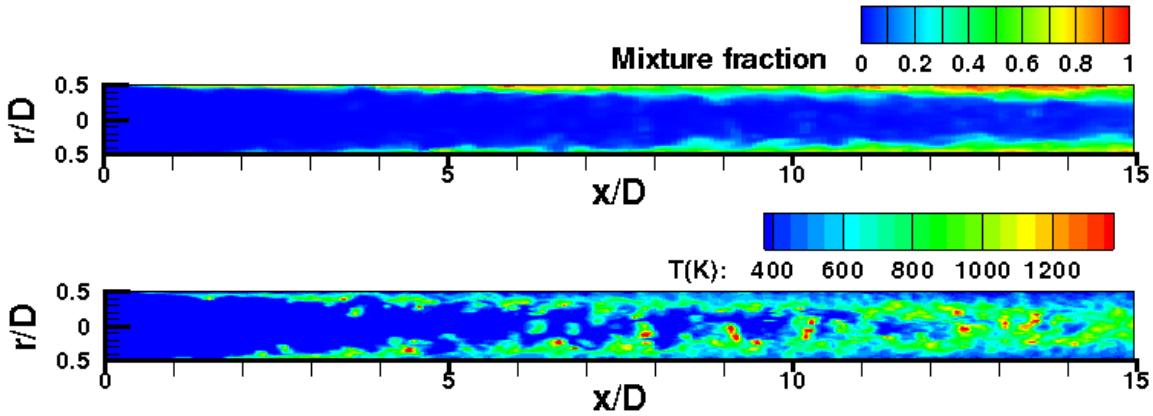


Figure F1: Mixture fraction (upper) and temperature (lower) snapshots

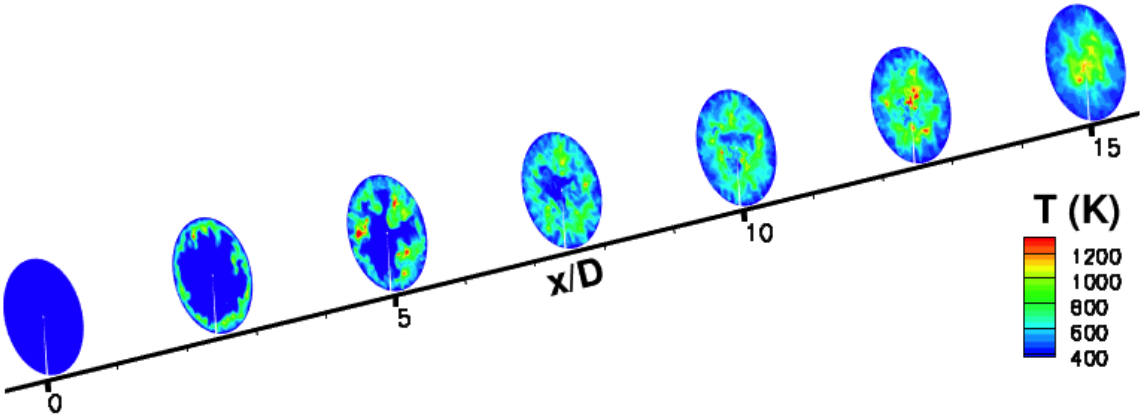


Figure F2: Reaction zone for several axial locations

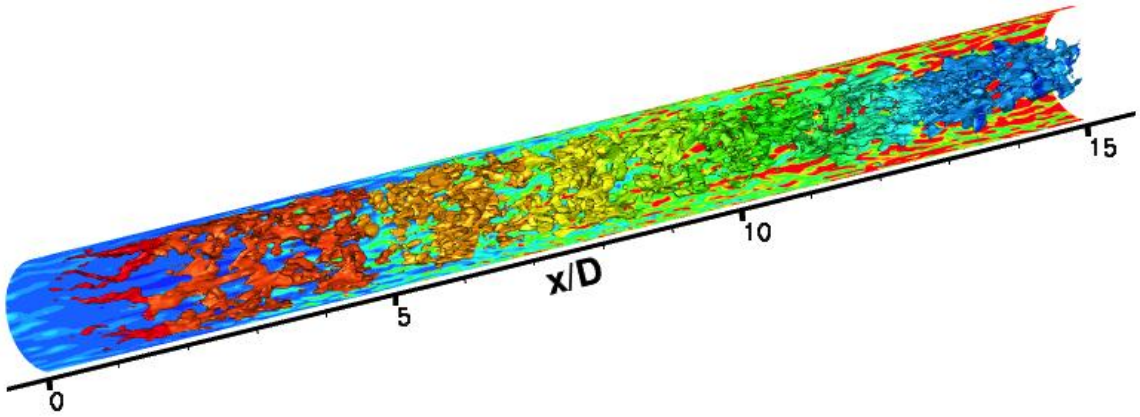


Figure F3: Isocontour of T=800K, along with axial velocity contour near wall.

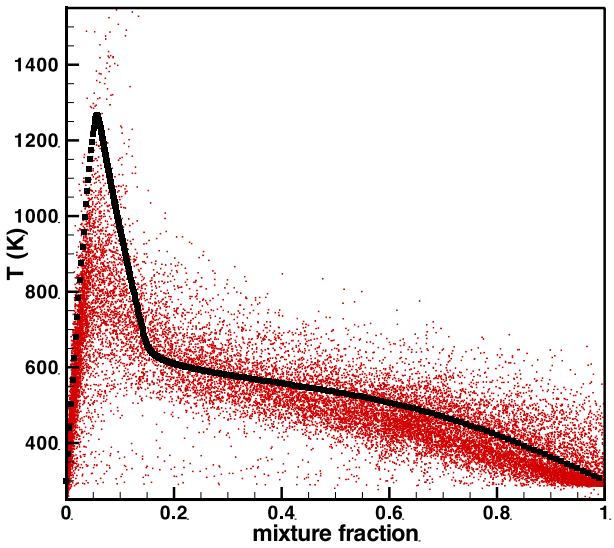


Figure F4: Scattered plot of temperature for mixture fraction, for all cells at an instant. Black dots follow equilibrium solution of the given fuel.

## References

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