

Fundamental Study toward Numerical Simulation of Turbulent Combustion Control

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Toward the numerical simulation of the total system of turbulent combustion control, fundamental studies on diffusion/premixed flames are conducted. In the diffusion flame simulation, the effect of swirled jet on the hydrogen/air jet diffusion flame is investigated and it is shown that the lift-off height decreases by the swirl effect. For premixed flame simulations, a non-reacting swirler flow is simulated and a one-dimensional analysis of combustion-driven oscillations is conducted. The swirler flow simulation demonstrated that the instantaneous flowfield is very turbulent and far from swirl flows but the time-averaged has a swirl flow feature. The one-dimensional computation of combustion-driven oscillation showed that the simulated pressure oscillation is surely combustion-driven and the phenomenon can be simulated by CFD if the boundary conditions are well-posed. It is shown that the combustion-driven oscillation is not large when the pressure disturbance does not affect the supply system, but it becomes very intense when the pressure disturbance affects the supply system and the mass flow rate gets resonant.

1. Introduction

The computational group for turbulent combustion control research at NAL (National Aerospace Laboratory) has been conducting fundamental analyses aiming at numerical simulations of total combustor systems that include smart control systems. The total system simulation will help us to construct efficient and clean combustion systems. To achieve this objective, the computational group has been developing simulation techniques and models, and trying to construct an intelligent database that helps us to extract knowledge efficiently from experimental and computational data.

In this fiscal year, the computational group mainly conducted numerical simulations of jet diffusion flames and preliminary studies for premixed flame simulations, that is, simulations of swirler flow and combustion-driven oscillation. In this paper, the results about diffusion and premixed flames are presented as follows.

Jet diffusion flame is an interesting research target itself and, in addition, it can be used as an actuator in premixed combustors. Hence, its control can be a key technology in constructing ideal combustors. In this paper, as a first step of control simulations, the effects of swirled jet injection on the hydrogen/air jet diffusion flame are investigated.

The objectives of the moment in premixed flame computation are to understand the flame holding mechanism and to conduct simulations of combustion-driven oscillations in a swirler combustor. Swirlers are very common premixed flame devices for flame holding. The flowfield of a non-reacting swirler flow is simulated to understand the flow structure and to pick out technical problems to be solved toward swirler combustor simulations. Combustion-driven oscillation is one of the most important and severest problems and has been studied for a long time. However, because the phenomenon strongly depends on the flow/reaction interaction and the systematic analysis has been quite difficult, the prevention method has been empirical so far and no general methodology has been established yet. Simulations of the phenomenon in combustors and invention of its prevention methods are major objectives of the numerical research. Takeno (1968) theoretically showed that the pressure fluctuation is driven by the fluctuation of heat release rate independently of the detailed reaction processes and that the phenomena can be predicted if the effects of flowfield on the heat release rate can be estimated. However, by theoretical approach, estimation of such effects is difficult and extension to real geometry combustors is also difficult. On the other hand, CFD (Computational Fluid Dynamics) approach has capability and flexibility to include all the flow/reaction interaction effects and possibility to predict combustion-driven oscillations. In this paper, as the first step, a one-dimensional numerical simulation by finite volume CFD is shown.

2. Diffusion Flame

Hydrogen/air jet diffusion flames have been simulated by DNS-like approach. The problem configurations are subject to the experiment by Cheng et al. (1992). A hydrogen jet is injected into still air at 680 m/sec, 0.54 in Mach number, from a round nozzle whose diameter D is 2mm, and a lifted flame of about 14mm lift-off height is obtained. The hydrogen/air chemical reaction model used for this simulation is the 9-species 17-reaction model by Westbrook (1982) and the Zel'dovich mechanism is coupled for NOx formation analysis. The grid spacing used for this simulation is about 2.5 times larger than the Kolmogorov scale around the ignition point. The total grid number is about 20 million. The details of the computational method should be referred to Mizobuchi and Ogawa (2000). The lift-off height in the numerical simulation is about 11mm and agreement is fairly good. The discrepancy seems to result from the gravity effect that is neglected in the computation. The gravity effect is now under investigation.

The effects of swirl injection are investigated here. The angular velocity is given so that the swirl velocity at the nozzle edge is 340m/sec. Figures 1: a) and b) show the temperature iso-surfaces at 1000K in normal and swirled injection cases, respectively. The lift-off height is about $1D$ shorter in the swirled case than the normal case. The close-up view of vortex structure near the nozzle exit is shown in Fig.2, where the iso-surfaces of the second invariant of velocity gradient tensor at a positive value are presented. The vortex structure becomes more complicated and the number of vortex tubes larger by the swirl. This change in the vortex structure enhances the momentum mixing between the hydrogen jet and air as well as the species mixing. The flame bottom is the position where the flow speed and the flame propagating speed balance. The increase of the momentum mixing makes flow deceleration rapider and the lift-off height shorter.

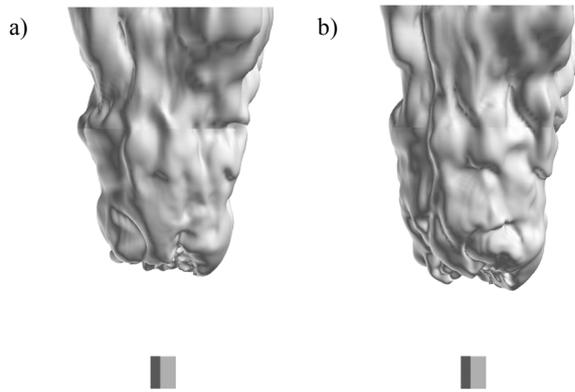


Figure 1: Iso-surface of temperature at 1000K, a): normal jet, b): swirled jet.

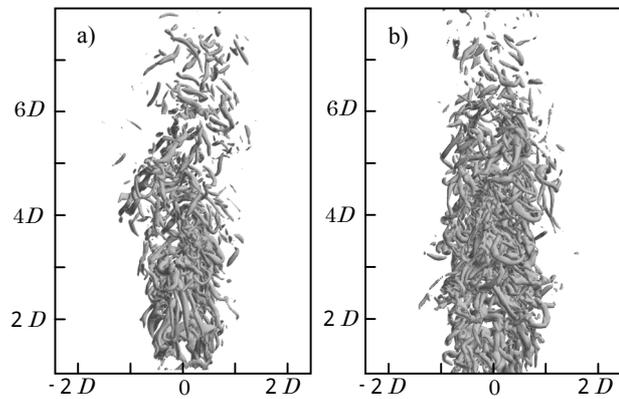


Figure 2: Iso-surface of the 2nd-invariant of velocity gradient tensor at a positive value, a): normal jet, b): swirled jet.

The swirl effects on other properties: combustion efficiency and NOx formation are not so significant. The momentum of the hydrogen jet is very small because hydrogen is so light compared with air. The effect of jet configuration modification cannot survive after being mixed with still air and therefore, cannot affect the chemical reactions.

3. Premixed Flame

One of the most important research topics is the flame instability such as combustion-driven oscillation in a premixed combustor, especially at a lean condition. The NAL experimental group is conducting experiments about a swirler combustor, which is a popular configuration for flame holding of premixed flames. The present goal of premixed flame simulation is to investigate the mechanisms of flame holding and combustion-driven oscillations in the combustor. For the purpose, as preliminary studies, two fundamental research elements are investigated here; one is a three-dimensional non-reacting swirl flow simulation and the other is a one-dimensional analysis of combustion-driven oscillation.

3.1 Swirler flow simulation

Swirlers are one of the most popular devices for premixed flames. The swirl effects produce recirculation regions that play an important role in flame holding. The authors are going to simulate combustion flows in swirler combustors, but at present, the computational resource at NAL is not enough to simulate the real-size reacting combustor flows. Considering the simulation on the next computer system, a non-reacting swirler flow has been simulated.

The schematic of the simulated swirler is shown in Fig.3. The coordinate system notations are subject to Fig.3 and the origin is the center of the swirler. The inner diameter D_i is 2mm, the outer D_o is 4mm, the vane angle Φ is 45 deg., and the model size is about one tenth of the experimental combustor. The

computational region is $-12D_i < x, z < 12D_i, 0 < y < 8D_i$. The grid system is rectangular, the grid spacing is 0.05mm around the swirler and the grid number used for this simulation is 8 million. In this simulation, the flowfield around swirler vanes is not solved and the swirler is treated just as a boundary. The boundary conditions are imposed as follows. On the swirler plane only the velocity direction is given according to the vane angle, independently of the vane number or vane configurations. The inlet velocity is extrapolated from the inside one-dimensionally in the second-order. The pressure and the temperature are calculated by supposing the adiabatic change from the reservoir state. The reservoir pressure is chosen to make the flow speed about 200 m/sec in order to keep the Reynolds number as large as that in the experiment. The Reynolds number based on D_i is about 100000. The inlet boundary condition is based on the one-dimensional steady theory and valid only when the inlet velocity is positive. Modification of the inlet boundary condition is needed in the future study.

Figure 4 presents the instantaneous vortex structure in the swirler flow. The iso-surfaces of the second-invariant of velocity tensor at a positive value are shown with the pressure distribution on the surfaces. So many vortex tubes exist and the structure is very complicated, which indicates that the flowfield is strongly turbulent. In this computation, no turbulence is explicitly imposed at any boundaries. The seed of the turbulence is numerical, but the evolution process yields to the Navier-Stokes equations.

Instantaneous velocity vectors on $y=\text{const.}$ planes are shown in Fig.5, a): $y=0$ (swirler surface), b): $y=3D_i$, c): $y=6D_i$. The color mapping shows the y -direction velocity component. The instantaneous velocity vectors look very random at $y=3D_i$ and especially at $y=6D_i$. This randomness shows the turbulence behaviour and corresponds to the complicated vortex structure shown in Fig.4. On the other side, the swirl flow feature is hardly observed in the instantaneous velocity vector fields and this computation does not look successful in simulating a swirler flow.

Figure 6 shows the velocity vectors obtained by time-averaging 14 samples over about 0.3msec. The time-averaged velocity vectors show the swirl flow feature. The x - z -direction velocity vectors rotate around the swirler centerline (the center of the figure), and the y -direction velocity component distribution is axisymmetric. On the $y=3D_i$ plane, a negative velocity region is observed near the swirler centerline, which indicates the existence of the recirculation region inside the rotating flow. This recirculation region is an advantageous feature of swirler flows that works to realize the flame holding in premixed combustion.

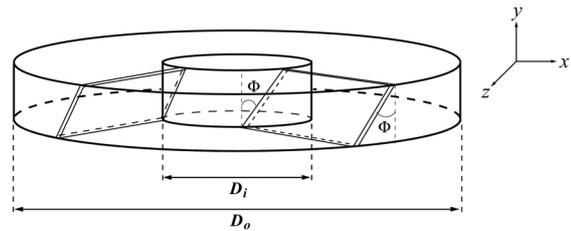


Figure 3: Schematic view of modeled swirler.

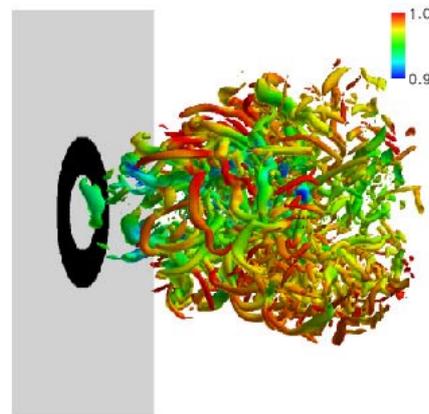


Figure 4: Iso-surface of the second-invariant of velocity gradient tensor at a positive value with pressure distribution.

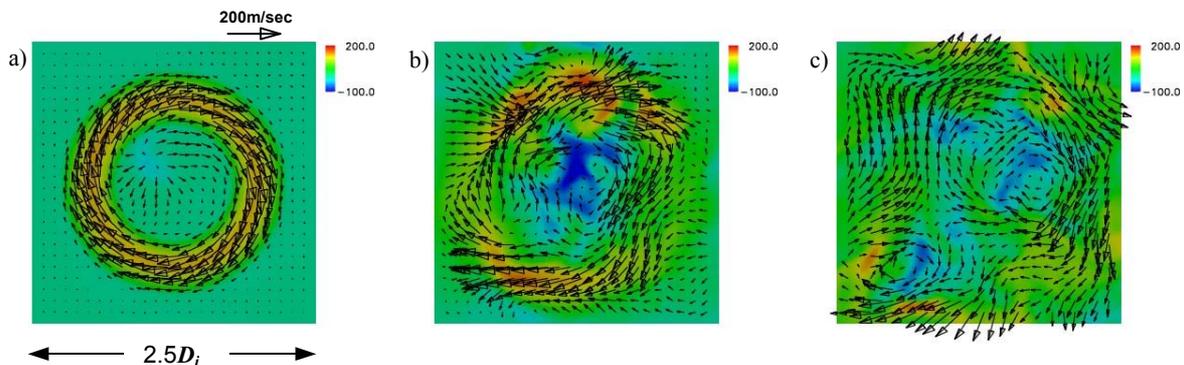


Figure 5: Instantaneous velocity vectors, a): $y=0$, b): $y=3D_i$, c): $y=6D_i$. Color mapping shows the velocity component perpendicular to the paper.

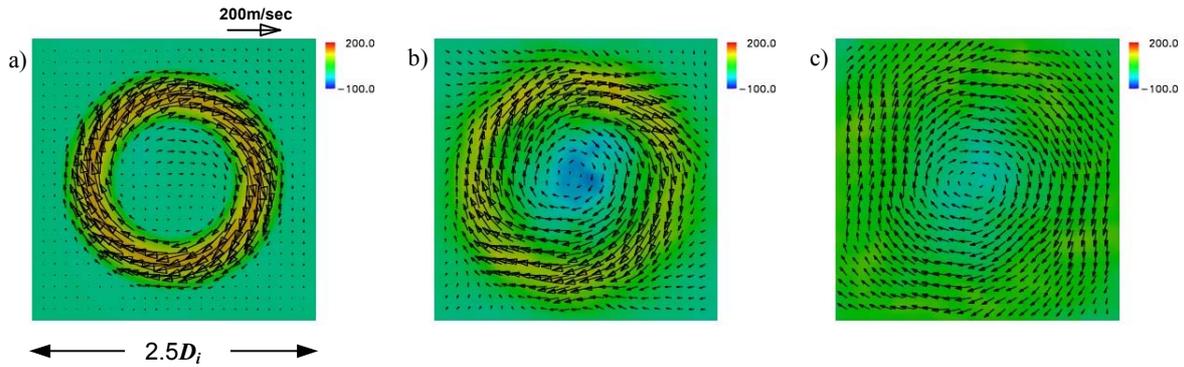


Figure 6: Time-averaged velocity vectors, a) $y=0$, b) $y=3D_i$, c) $y=6D_i$. Color mapping shows the velocity component perpendicular to the paper.

The computation of the turbulent swirler flow conducted here shows a very random feature in the velocity field that is far from swirler flows in instantaneous states, but simulates reasonably the swirler flowfield in the time-averaged state.

3.2 One-dimensional analysis of combustion-driven oscillation

Combustion-driven oscillation is driven by the heat release rate fluctuation [Takeno (1968)] and strongly amplified when the fluctuations of heat release rate, pressure and mass flow rate are in resonance. To simulate such phenomena in combustors, pressure propagation in the combustor, reflection at the boundaries and the heat release rate response to the flowfield conditions should be properly simulated numerically. From the viewpoint of CFD technique, the discretization method should be accurate and the boundary conditions have to be well-posed.

Here, one-dimensional analysis is conducted to examine the computational technique, to find out problems to be solved and to understand the phenomenon. The schematic of the simulation is shown in Fig.7. Premixed gas comes from an infinitely large reservoir, burns in a one-dimensional tube, and then goes out into a constant-pressure atmosphere. The discretization method is based on a finite volume method and the convective terms are evaluated with a TVD numerical flux based on Roe's scheme [Roe (1981), Wada et al. (1989)], which keeps higher-order even in regions where the sign of a physical quantity's gradient changes [Wada (1995)]. At the inlet boundary the velocity is extrapolated in the second order, and the total pressure and the total temperature are fixed at the values in the reservoir. At the exit boundary the static pressure is fixed at a value that is properly chosen to keep the flame front in the computational region. At the initial condition, the left half of the computational region is in the reservoir conditions and the right half in the adiabatic flame conditions.

The tube length is 20mm. The premixed gas is 40% hydrogen + air, and the temperature and the pressure are 328K and 1atm, respectively. The chemical reaction model is the same that used in the jet diffusion flame computations. In this condition, the simulated flame speed is about 4.4m/sec, which shows good agreement with measured flame speed: 4.2m/sec [Abdel-Gayed et al. (1984)], but the oscillation is not so large. Hence, in order to make the problems clear, the model simulations are conducted using ten times faster reaction rates.

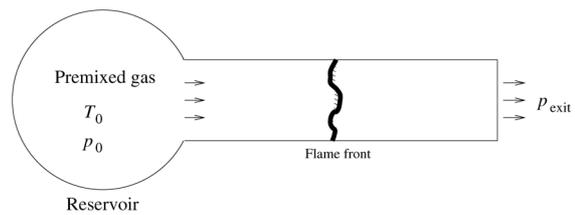


Figure 7: Schematic of 1-D model simulation of combustion-driven oscillation.

Figure 8 shows the instantaneous distributions of physical properties in a stable oscillation case. The distributions of temperature, gauge pressure (difference from the exit pressure), velocity, density and heat release rate are drawn in red, blue, orange, yellow and green lines, respectively. An oscillation is observed in the burned region, which has a node at the tube exit and the wavelength of which is about one-third of the distance between the flame front and the tube. In the unburned region, the wavelength is about one-seventh, but the oscillation decays as the distance from the inlet boundary decreases. The information of the pressure fluctuation hardly arrives at the gas supply system, and the resonance between the pressure oscillation and the mass flow rate is not so significant in this case. Numerical dissipation may attenuate the oscillation, but this oscillation decay is mainly due to the inlet boundary condition. The inlet boundary condition allows negative pressure fluctuation freely but binds the positive fluctuation because the total pressure is fixed and the upper limit of the pressure is defined. Hence, the inlet boundary condition has an effect of damping the oscillation. The spectrum analysis of the pressure fluctuation is shown in Fig.9. A

peak lies around 300KHz. This frequency corresponds to the period during which the sound travels the wavelength in both regions: unburned and burned regions. In this case, the period (wavelength /sound speed) is almost the same in both regions. The sound speed is 461 m/sec and 1074 m/sec in the unburned and the burned regions, respectively.

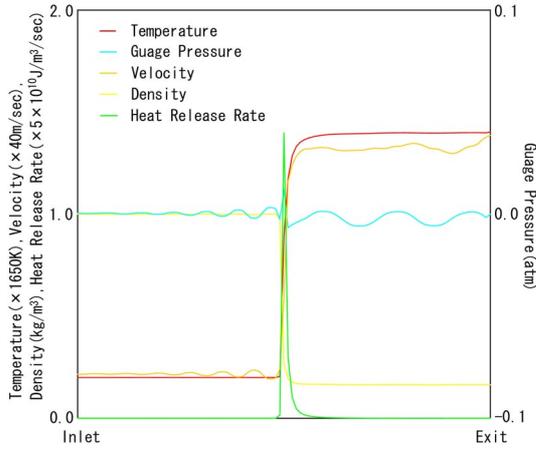


Figure 8: Distributions of physical properties in 1-D tube.

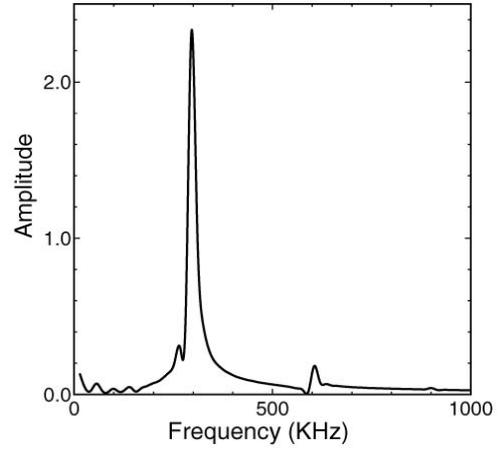


Figure 9: Pressure oscillation spectrum.

The Reyleigh criterion is known as a necessary condition for combustion-driven oscillations. The condition is written as [Reyleigh (1945), Putnam and Dennis (1954)],

$$W = \oint p' \dot{q}' dt > 0 ,$$

where p' and \dot{q}' are the fluctuations of pressure and heat release rate, respectively. Figure 10 shows the time histories of the pressure and heat release rate fluctuations. In this case, $W = 1.33 \times 10^5 \text{ [J}^2/\text{m}^6/\text{sec}] > 0$ and therefore it can be concluded that this pressure oscillation is not a numerical oscillation, but a combustion-driven oscillation that is driven by the heat release rate fluctuation.

The oscillation characteristics depend on the initial perturbations, the gas conditions, the flame front position in the computational region and so on. In the above case, the pressure fluctuation does not affect much the inlet boundary. Depending on the conditions, solutions in which the pressure oscillation affects much the inlet boundary and the mass flow rate resonates can be obtained. Instantaneous physical properties' distributions in such a case are shown in Fig.11. The difference between the results shown in Fig. 8 and 11 is the time stepping in the early time. In the latter case, the initial time step is larger and the numerical disturbance is larger, and the large pressure disturbance arrives at the inlet boundary. Once the pressure perturbation arrives at the inlet and the mass flow rate gets resonant, the oscillation becomes larger and more complicated. Moreover, eventually the inlet velocity becomes negative, and then, the simulation breaks down. The oscillation is very sensitive to the initial perturbation, and the oscillation becomes very intense in the cases where the supply system is in resonance.

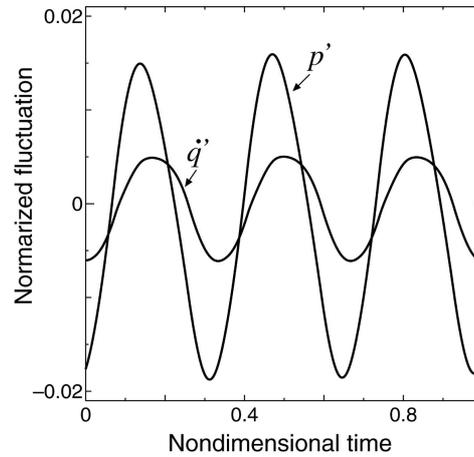


Figure 10: Time histories of pressure and heat release rate fluctuations.

As mentioned in the swirler flow section, the inlet boundary conditions used here presume steady flows and are valid only when the inlet velocity is positive. When the oscillation at the inlet boundary becomes large, the validity of these assumptions may not be guaranteed. The consideration about the inlet boundary condition is needed in the future study.

4. Concluding Remarks

As fundamental studies toward the total system simulations of turbulent combustion control, jet

diffusion flame, swirler flow and combustion-driven oscillation are investigated and following major conclusions are obtained.

- The lift-off height of a hydrogen/air jet diffusion flame decreases by the swirled injection effects, because the swirl increases the turbulence and enhances the momentum mixing between hydrogen jet and air, and thus the jet speed deceleration becomes rapider.
- A three-dimensional swirler flow is simulated. The instantaneous flowfield shows a very random and turbulent feature that is far from a swirl flow, but the time-averaged flowfield shows the typical swirl flow features: rotating velocity vectors and recirculation region inside the rotating flow.
- One-dimensional numerical model simulations of combustion-driven oscillations are conducted.
 - The simulated pressure oscillation satisfies the Reyleigh criterion and it is a combustion-driven oscillation.
 - The simulated wavelength and frequencies of the oscillation are characterized by the sound speed and the lengths of unburned and burned regions.
 - The oscillation is very sensitive to the initial perturbation and becomes very intense when the mass flow rate gets resonant.

In all computations shown here, the treatment of the inlet boundary condition is the most important and annoying problem. The investigation into the inlet boundary condition is indispensable in order to advance the total system simulations of combustion flows.

The computational group is going to integrate the numerical results and knowledge obtained during this fiscal year to realize the total system simulations of turbulent combustion flow control. The control devices may be MEMS, loud speakers, micro jets, mass rate controllers and so on. The simulation of the effects of such control devices must be included in the system simulations.

In addition, the group is constructing a knowledge database that utilizes the network and enables the seamless data interchange between different types of data of different kinds of researchers. Using the database, the results of experiments and numerical simulations will be organically processed, and the knowledge needed to establish the turbulent combustion control scheme will be extracted.

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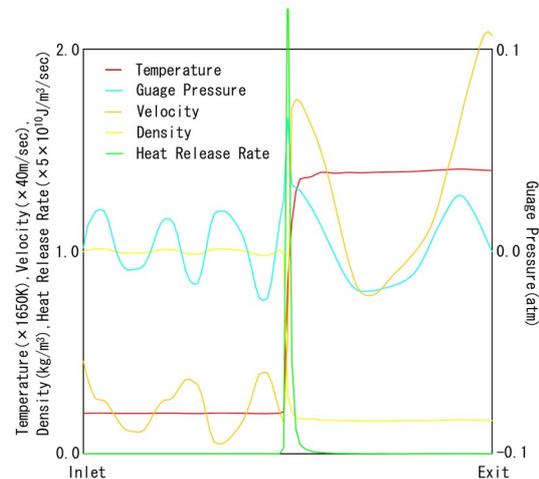


Figure 11: Distributions of physical properties in 1-D tube in case that the supply system is in resonance.