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Large-eddy simulation of a supercritical channel flow using a shock capturing numerical scheme

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ABSTRACT

This paper investigates the simulation of supercritical fluids flowing inside small cooling channels. In the context of liquid rocket engines, a strong heat flux coming from the combustion chamber (locally $\phi \approx 80$ MW/m^2 for the Ariane 5 main-engine) may lead to very steep density gradients close to the wall. These gradients have to be thermodynamically and numerically captured to really understand the mechanism of heat transfer from the wall to the fluid. A shock-capturing WENO numerical scheme, usually used with the ideal gas law, was extended to real gases and applied to the simulation of an academic channel flow configuration that uses hydrogen as fluid. Results showed very elongated ligaments in the streamwise direction with a deep penetration in the wall-normal direction. A linear analysis was performed to link the fluctuations of compressibility factor (Z') to temperature fluctuations (T') in the case of an adiabatic and isothermal wall. The usual Strong Reynolds Analogy (SRA) could not be confirmed with real gas effects. Z fluctuations was found lower than 1%, thus becoming harder to distinguish the physical fluctuations from the numerical error and a more refine simulation should be require to deliver a definitive conclusion.

1. Introduction

The ability to model and predict heat transfer of wall-bounded compressible turbulent flows is crucial in the design and optimization of aerospace propellants. In particular, when increasing the thrust efficiency of future liquid rocket engines (LRE), the combustion chamber must operate at very high pressures and temperatures. This requires sufficient cooling to maintain the chamber walls within acceptable temperature limits either to prevent failure or increase cycle life. For instance, the nonlinear deformation of the combustion chamber wall has been studied by Riccius et al. [1] under cyclic thermal and mechanical loading. Regenerative cooling or forced convection cooling are the most common methods used: a cryogenic fuel in a supercritical state, typically H_2, flows in small channels embedded in the chamber walls, including the nozzle throat portion, and absorbs the heat from the hot-gas side wall. For such configurations, experiments over the past ten years have shown a significant thermal-load sensitivity to channel size, geometry effects and fluid properties. For example, the use of high aspect ratio (height/width) cooling channels (HARCC) [2,3] is a promising technique to reduce the near wall combustion chamber temperature for a limited pressure drop. For example, the effect of tube geometry on regenerative cooling performance has been studied by Parris and Landrum [4], and Pizzarelli et al. [5,6] simulated the behavior of supercritical fluids inside heated curved channels in a RANS (Reynolds-Averaged Navier–Stokes) context. They observed the existence of strong fluid recirculation contrary to the straight channel case. According to the authors, there is no large-eddy simulation (LES) of such configuration.

The description of a turbulent flow passing through narrow channels and experiencing a strong heat transfer involving large compressibility effects is still a numerical challenge. Much efforts are then required to put emphasis into the near-wall thermal structures and their impact on the mean velocity and temperature distributions. Based on the wall-normal vorticity contours, Coleman et al. [7] have shown the existence of long and coherent streaks close to the wall and under strong compressibility effects as well as horseshoe-like (HS) structures. These latter are classical structures for channel flow configurations and have already been observed in sub- and super-sonic [8,9] configurations. The HS structure is strongly three-dimensional and is a key-factor of the heat exchange between the cold and the hot parts of flow [10].

In contrast to this very precise analysis, the engineering design of LRE cooling systems requires correlations to predict the heat

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transfer from the burned gases to the combustion chamber wall, and from the wall to the cooling fluid. Such a study for supercritical hydrogen in regenerative cooling channels has been recently done by Locke and Landrum [11]. Pioro et al. [12] have detailed similar correlations in the context of supercritical water for fossil-fired power plants. Finally, Cheng et al. [13] studied the heat transfer in supercritical water cooled flow channels in the context of nuclear power plant design.

The objective of the present paper is to study the supercritical fluid behavior in a LRE cooling channel by using numerical computations. To achieve this objective a numerical scheme based on WENO (Weighted Essentially Non-Oscillatory) formulation is developed for general fluid flows, i.e. regardless the equation of state. Indeed, such strategy may be crucial to capture the large density gradient that may be found when studying the supercritical fluid flows [14]. Appropriated thermodynamics relations required to deal with real gas effects are also presented in the next section. In Section 3, the channel flow configuration is detailed and results are analyzed. Conclusions are provided in Section 4.

2. Thermodynamics and numerical solvers

Simulating a supercritical flow requires a unified treatment of general fluid thermodynamics, valid for the entire state of fluid [15]. For instance, Yang and coworkers [15–19] developed and validated various numerical codes able to simulate different configurations: droplet vaporization, laminar diffusion flames, supercritical fluid injection, mixing, swirl injector, *etc.* Characteristics of the LES numerical code that were used in the present study may be found in Zong and Yang [19]. Nevertheless, it is useful to note that a preconditioning scheme is applied to simulate either sub- or super-sonic flows and that the spatial discretization is achieved with a fourth-order, central-difference scheme (acronym 4CD) in generalized coordinates. A dual-time-stepping integration technique [15] is used with a standard fourth-order Runge–Kutta scheme to perform the inner-loop pseudo-time integration and a second-order backward difference for the real-time derivative term [20]. To ensure computational stability and to prevent numerical oscillations in regions with steep gradients, a fourth-order scalar dissipation with a total-variation-diminishing switch developed by Swanson and Turkel [21] is used. This strategy may be too dissipative as it will be shown in Section 2.2, and a WENO formulation is derived for general fluids hereafter according to the procedure given by Jiang and Shu [22]. Note that the WENO formulation of Martin et al. [23] allows a dynamic balance between a quasi-full-upwind formulation for steep gradients regions and a quasi-central formulation in smooth regions.

2.1. WENO formulation for general fluid flow

Developing a numerical scheme for general fluid flow requires particular attention to partial derivatives due to the numerical stiffness caused by rapid flow property variations. The differential form of the internal energy $e = e(T,\rho)$ may be expressed as

$$de = \left(\frac{\partial e}{\partial T}\right)_\rho dT + \left(\frac{\partial e}{\partial \rho}\right)_T d\rho = C_v dT + C_T d\rho, \tag{1}$$

where T and ρ are temperature and density, respectively. The differential form of specific enthalpy $h = e + p/\rho$ is written

$$dh = de + \frac{dp}{\rho} - \frac{p}{\rho^2}d\rho = C_v dT + \left(C_T - \frac{p}{\rho^2}\right)d\rho + \frac{dp}{\rho}, \tag{2}$$

where p is pressure. Introducing the differential form of temperature $T = T(p,\rho)$, Eq. (2) can be written

$$dh = \left[C_v\left(\frac{\partial T}{\partial \rho}\right)_p + C_T - \frac{p}{\rho^2}\right]d\rho + \left[C_v\left(\frac{\partial T}{\partial p}\right)_\rho + \frac{1}{\rho}\right]dp. \tag{3}$$

A similar derivation may be done to express the differential form of the specific enthalpy as a function of temperature and pressure. This leads to:

$$\begin{aligned} dh &= \left[C_v + \left(\frac{\partial \rho}{\partial T}\right)_p\left(C_T - \frac{p}{\rho^2}\right)\right]dT \\ &\quad + \left[\left(\frac{\partial \rho}{\partial p}\right)_T\left(C_T - \frac{p}{\rho^2}\right) + \frac{1}{\rho}\right]dp, \qquad (4)\\ &= C_p dT + C_{T'} dp. \qquad (5) \end{aligned}$$

Introducing C_p (Eq. (5)) into Eq. (3) leads to the differential form of h:

$$\begin{aligned} dh &= C_p\left(\frac{\partial T}{\partial \rho}\right)_p d\rho + \left[C_v\left(\frac{\partial T}{\partial p}\right)_\rho + \frac{1}{\rho}\right]dp, \qquad (6)\\ &= \left(\frac{\partial h}{\partial \rho}\right)_p d\rho + \left(\frac{\partial h}{\partial p}\right)_\rho dp. \qquad (7) \end{aligned}$$

To capture the steep density gradients that are inherent to supercritical flows, a WENO formulation was adopted. This procedure can be applied to any system of hyperbolic conservation laws after their transformation from physical to characteristic space [22]. The transformation requires a special attention to partial derivatives and thermodynamics laws. To highlight this point, the WENO method for general fluids is described in the context of the scalar one-dimensional advection equation,

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial x} = 0, \tag{8}$$

where $W = [\rho, \rho u, \rho e_t]^T$ is the conservative variables vector. $F = [\rho u, \rho u^2 + p, (\rho e_t + p)u]^T$ represents the conservative variables flux vector. u and e_t are velocity (the velocity components are $\{u, v, w\}$) and specific total energy, respectively. Introducing the vector of primitive variables $V = [\rho, u, p]^T$ into Eq. (8) leads to:

$$\frac{\partial V}{\partial t} + \widetilde{A}\frac{\partial V}{\partial x} = 0, \tag{9}$$

where $\widetilde{A} = M^{-1}AM$ with $A = BM^{-1}$. The jacobian matrices $M = \partial W/\partial V$ and $B = \partial F/\partial V$ are expressed as,

$$M = \begin{bmatrix} 1 & 0 & 0 \\ u & \rho & 0 \\ \alpha & \rho u & \beta \end{bmatrix}, \tag{10}$$

and

$$B = \begin{bmatrix} u & \rho & 0 \\ u^2 & 2\rho u & 1 \\ u\alpha & \rho e_t + p + \rho u^2 & (\beta+1)u \end{bmatrix}, \tag{11}$$

where $\alpha = \partial(\rho e_t)/\partial\rho|_{u,p}$ and $\beta = \partial(\rho e_t)/\partial p|_{u,\rho}$. The total energy, e_t, may be split into a specific internal energy, e, and a kinetic energy, $e_c = u^2/2 : e_t = e + e_c$. The matrix A is then written as,

$$A = \frac{1}{\beta\rho}\begin{bmatrix} 0 & \beta\rho & 0 \\ \rho(u^2 - \alpha + \beta u^2) & \rho u(2\beta - 1) & \rho \\ -u(\rho\beta e_t + \beta p - \rho u^2 + \rho\alpha) & \beta\rho e_t + \beta p - \rho u^2 & \rho u(\beta+1) \end{bmatrix}, \tag{12}$$

leading to