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Modeling supercritical heat transfer in compressible fluids

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A B S T R A C T

Novel solutions have been derived for both thermodynamic and hydrodynamic models of the heat transfer inside a cavity containing supercritical fluid in zero gravity. A fully analytical solution of the thermodynamic model was obtained through a combination of the Generalized Integral Transform Solution and the Matrix Exponential Method. Its accuracy is entirely controlled by a single user prescribed parameter. Furthermore, a low Mach Preconditioned Density-Based Method was employed to generate a numerical solution of the hydrodynamic model, avoiding acoustic filtering and the need to resolve acoustic time scales without it. A proper model for the piston effect evolution in pseudo-time must be included to generate a physically correct description of its physical-time evolution. Furthermore, both models generate graphically identical results, but only upon a thermodynamically consistent selection of fluid properties and equation of state. Finally, the theoretical expression for the piston effect relaxation time underestimates the actual value of this characteristic time estimated from a simulation of the same model used to derive this expression. This feature is not an artifact of boundary condition choice.

1. Introduction

All fluids are subject to a universal divergence of their thermodynamic properties as their critical points are approached. Even though the thermal diffusion relaxation time diverges near the critical point, a very fast temperature equilibration is still observed in enclosed samples on both ground-based [1] and microgravity [2] experiments. Such a critical speeding-up has been explained using simulations of a thermodynamic model [3,4] as well as a hydrodynamic model [5]. It is caused by the ability of small temperature perturbations to create severe compression in near-critical fluids, which generates thermo-acoustic waves. When entrapped within cavity walls, their propagation and reflection induces a rapid heating of the entire fluid, resulting in a homogeneous increase of its bulk temperature. This fast temperature relaxation phenomenon is known today as piston effect and it has been the subject of several reviews in the literature [6–9].

The original thermodynamic model developed for supercritical heat transfer under microgravity conditions [4,3] is essentially the heat conduction equation with a source term proportional to the bulk temperature time derivative. This source term models the adiabatic compression mechanism responsible for the piston effect. It becomes dominant whenever $\gamma \gg 1$, i.e. closer to the critical point. On the other hand, it vanishes in the incompressible limit, where $\gamma = 1$. A solution to this equation, including variable properties obtained from available data in the literature, was first generated with numerical methods [4]. However, bulk temperatures are obtained by numerical integration of the temperature field over the entire simulated volume at each time step. Such an approach can become costly for two and three-dimensional domains. In order to circumvent this problem, an alternative approach was proposed that replaces the volume integral by a surface integral using the Boundary-Element Method [10]. An additional solution to this equation, now considering constant properties, was first obtained with an approximate Fourier transformation procedure [3], where a detailed derivation is provided elsewhere [11]. Although both studies considered steady heating at the boundaries, the approximate Fourier procedure has been extended towards pulsed [12] and unsteady [13] heating as well. The original work [11] also considered a conjugate problem, coupling the thermodynamic model for the fluid with a heat conduction model for the solid walls containing a composite material. It was extended later to include curvature effects due to cylindrical container walls [14], although a different approximate analytical approach was utilized. Separation of variables was applied to the solid wall heat conduction problem whereas a Laplace transform with numerical

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Nomenclature

$\widehat{\mathbf{A}}$	inviscid flux Jacobian based on primitive variables matrix
$\mathbf{A}$	integral transformed matrix
$A_{i,j}$	integral transformed matrix coefficient
$\mathbf{B}$	integral transformed matrix
$B_{i,j}$	integral transformed matrix coefficient
BDF	backwards difference formula
c	sound speed
$\widehat{c}$	preconditioned sound speed
C_P	specific heat at constant pressure
C_V	specific heat at constant volume
e	internal energy per unit mass
E	total internal energy per unit mass
$\mathbf{E}_i$	inviscid flux vector
$\mathbf{E}_v$	viscous flux vector
$\mathcal{F}$	dimensionless temperature filter
h	enthalpy per unit mass
h_P	preconditioned enthalpy Jacobian with respect to temperature
h_T	preconditioned enthalpy Jacobian with respect to pressure
H	total enthalpy per unit mass
$\mathbf{H}$	source term vector
k	thermal conductivity
L	cavity length
$\widehat{\mathbf{M}}$	preconditioned inviscid flux Jacobian matrix
Ma	Mach number
N	number of terms in summation series solution
N_i	norm
N_T	number of terms in temporal grid
N_x	number of terms in spatial grid
P	pressure
P_H	hydrodynamic pressure
P_T	thermodynamic pressure
$\mathbf{Q}$	conservative dependent variable vector
$\widehat{\mathbf{Q}}$	primitive dependent variable vector
t	physical-time coordinate
t_D	thermal diffusion relaxation time
t_{PE}	piston effect relaxation time
T	temperature
$\mathbf{T}$	conservative to primitive dependent variable Jacobian matrix
u	velocity
x	spatial coordinate

Greek symbols

α	thermal diffusivity
α_P	isobaric thermal expansion coefficient
β_i	eigenvalue
δ	increment
$\delta_{i,j}$	Kronecker delta
Δ	absolute error
ε	preconditioned sound speed control parameter
η_i	integral transform coefficient
γ	ratio between specific heats
$\mathbf{\Gamma}$	preconditioning matrix
κ_T	isothermal compressibility
μ	dynamic viscosity
ψ_i	eigenfunction
$\tilde{\psi}_i$	normalized eigenfunction
θ	homogeneous dimensionless temperature
$\bar{\boldsymbol{\theta}}$	integral transformed homogeneous dimensionless temperature vector
$\bar{\theta}_i$	integral transformed homogeneous dimensionless temperature
Θ	dimensionless temperature
Θ_b	dimensionless bulk temperature
ρ	density
ρ_P	preconditioned density Jacobian with respect to temperature
ρ_T	preconditioned density Jacobian with respect to pressure
τ	dimensionless pseudo-time coordinate
τ_{PE}	dimensionless piston effect relaxation time
ξ	dimensionless spatial coordinate

Subscripts

0	initial state, right wall
1	left wall
b	bulk state
c	critical point
D	thermal diffusion
H	hydrodynamic
i	series summation index
j	series summation index
P	isobaric
PE	piston effect
T	isothermal, thermodynamic
V	isovolumetric

inversion was applied to the supercritical fluid problem. Recently, the Generalized Integral Transform Technique was applied to a variation of this thermodynamic model where all fluid properties have a linear dependence on both temperature and pressure [15], confirming that variable properties have little impact on the bulk temperature evolution [16]. This hybrid technique analytically transforms the thermodynamic model into an unsteady system of ordinary differential equations, which is then numerically marched forward in time.

Such simplified models are able to predict bulk temperature and density evolutions on piston effect and thermal diffusion time scales, respectively [10]. However, pressure is space averaged since the speed of sound is assumed much faster than any other local fluid speeds. If an accurate description of supercritical heat transfer is desired on acoustic time scales, the propagation of pressure waves must be resolved [9], as demonstrated in early studies using a hydrodynamic model [5]. This particular model solved the Navier–Stokes equations coupled with the van der Waals equation of state using the PISO method [17]. Improved numerical results at both acoustic and thermal diffusion time scales have been obtained from this model for single [18,19] and binary [20] supercritical fluids using the explicit Mac-Cormack method with the FCT algorithm [21] to minimize spurious numerical oscillations. The same method has also been applied to an alternative version of the above hydrodynamic model for supercritical fluids [22–24] that uses instead a real gas equation of state as well as characteristics-based boundary conditions [25]. This model was solved recently using a Crank–Nicolson scheme for temporal discretization and a central differences scheme for spatial discretization [26], coupling velocity and