FSI-11-TN58Rev

Modeling Thermal Expansion Effects in *FLOW-3D*®

C.W. Hirt
Flow Science, Inc.
08/09/01, Revised 07/05/11

This Technical Note describes the modeling method used in ***FLOW-3D***® for thermal expansion processes in a one-fluid, incompressible flow. A typical approximation, when density changes caused by temperature variations are small, is to ignore actual volume changes and simply define the density as a function of temperature. This works well in many situations including natural convection caused by modest temperature variations.

If volume changes corresponding to density changes are important, then a somewhat more complicated model must be used. Furthermore, some attention must be given to the distinction between confined and unconfined flows when volume changes occur.

In the following discussion it will be assumed that density variations caused by temperature have a linear dependence on the temperature. In particular, if ρ is the density, T is temperature and β denotes the thermal expansion coefficient,

$$\rho = \rho_0 \left(1 - \beta \left(T - T_0\right)\right). \tag{1}$$

In this expression ρ_0 is the density at $T=T_0$, a reference temperature.

In the simplest approximation, mentioned in the introduction, an incompressible fluid would continue to satisfy the condition of incompressibility, which is the vanishing of the divergence of the velocity (i.e., a zero rate of change of volume),

$$\nabla \bullet \vec{u} = 0 . \tag{2}$$

The density would be evaluated using Eq.1, resulting in buoyant forces associated with a variable density.

When actual volumetric changes arising from changes in density are to be computed then the proper model equations to be satisfied can be derived from the assumption of conservation of mass. Written in an Eulerian form, mass conservation implies that

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \rho \vec{u} = 0 . \tag{3}$$

For present purposes we expand the divergence term and introduce the "derivative following the fluid" d/dt to rewrite this equation,

$$\frac{d\rho}{dt} + \rho\nabla \bullet \vec{u} = 0, \qquad \textbf{where} \qquad \frac{d\rho}{dt} \equiv \frac{\partial\rho}{\partial t} + \vec{u} \bullet \nabla\rho \tag{3a}$$

The derivative following the fluid means the time rate of change in density of a particle of fluid as it moves about. Because it refers to a particular particle, and we assume that density is a function of pressure, p, and temperature, we can write,

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial p}\frac{dp}{dt} + \frac{\partial\rho}{\partial T}\frac{dT}{dt} \tag{4}$$

Finely, using thermodynamic relations, $\partial p/\partial\rho = c_s^2$, where c_s is the speed of sound in the fluid, and $\partial\rho/\partial T = -\rho_o\beta$, which comes from Eq.1, we have,

$$\frac{1}{\rho_0 c_0^2}\frac{dp}{dt} + \nabla \bullet \vec{u} = \beta\frac{dT}{dt}\ . \tag{5}$$

This is the desired extension of the incompressibility condition Eq.2 that incorporates density changes from thermal expansion effects (right hand side) as well as from fluid compressibility (first term on left hand side). Although it was stated at the beginning that only a linear dependence of density on temperature was our objective, we could consider β in Eq.5 to be a function of T, which would allow for more general temperature dependence.

To include a thermal-expansion volume source (right side of Eq.5) in computations it is necessary to set an input flag *ifthexp*=1, which can be done through the Graphical User Interface. In most cases the compressibility term is not important, except for confined flow as discussed below.

In ***FLOW-3D®*** the actual density value is computed from Eq.1 or from a table of temperature vs. density values. Fluid velocities are then advanced in time by one time step δt, except for pressures, which are to be evaluated at the advanced time. The advanced pressures needed to complete the solution are computed from Eq.5 by treating the velocity to be a function of pressure so as to satisfy the modified compressibility condition.

When a flow is not confined Eq.5 indicates that a rise in temperature corresponds to a positive velocity divergence (assuming $\beta > 0$), which means an increase in fluid volume, although the overall mass of the fluid should not change.

Because we track fluid using a volume of fluid technique (TruVOF™) we must modify the computation of the volume of fluid function F so that it will remain unity in the interior of the fluid, but increase elsewhere to account for the volume change.

The basic equation for the fractional volume of fluid function, *f*, is a simple advection equation

$$\frac{\partial f}{\partial t} + \vec{u} \bullet \nabla f = 0 \qquad (6)$$

In the interior of a fluid, where f=1, this equation will not change the value of f. As a check on accuracy, ***FLOW-3D***® does not use Eq.6, but a instead uses a conservative formulation,

$$\frac{\partial f}{\partial t} + \nabla \bullet \left(f\vec{u} \right) = 0 \,. \qquad (6a)$$

This equation will reveal changes in f if the velocity divergence, Eq.2, is not satisfied and this provides a useful check on the accuracy of incompressible flow simulations.

When Eq.2 is replaced by Eq.5 for compressible or thermally expandable effects, then the fluid fraction equation must be changed accordingly,

$$\frac{\partial f}{\partial t} + \nabla \bullet \left(f\vec{u} \right) = f\left(-\frac{1}{\rho_0 c_s^2}\frac{dp}{dt} + \beta \frac{dT}{dt} \right). \qquad (6b)$$

When the divergence satisfies Eq.5, then Eq.6b reduces to Eq.6, which makes it consistent with the fluid fraction concept.

Confined Flow

Density is evaluated according to Eq.1 for purposes of evaluating buoyancy forces, however, the actual density variable is not changed unless there is an actual expansion or contraction in the flow. Thus, the total mass, which is computed in terms of density, will not change in a confined flow situation.

In a confined flow the integrated velocity divergence over the entire flow must be zero. This means that if the temperature increases anywhere in the flow, without a corresponding decrease in temperature then Eq.5 will have a solution only if the compressible term (first term) is not zero. In this case a pressure increase (compression) must compensate for the lack of volume expansion.

Unconfined Flow

In unconfined flows the pressure does not have to completely compensate for all density changes. A small pressure increase is associated with a local increase in temperature because it is needed to generate velocities directed away from the hot spot that decreases the density. This happens even if there is no compressibility in the fluid because of Eq.5, however, Eq.6b insures that f will remain at f=1.0 to indicate a fully occupied fluid region.

Testing These Results

Two simple one-dimensional tests have been conducted to check the assertions in the previous discussion. The first test is a column of fluid 10.0cm high confined by rigid walls. The second test is a column of fluid 10.0cm high with a free top surface. There is no gravity in either test. A power source was placed in the fluid that increases its temperature by 1.0° per second. The computations were run for 1.0s and all cases used the thermal expansion option, *ifthexp*=1.

Fluid properties are those of water in cgs units:

Density=1.0
Viscosity=0.01
Specific Heat=4.187e7
Thermal Conductivity=6.5e4
Thermal Expansion Coefficient=0.0003
Reciprocal bulk modulus=4.3e-11 (based on a sound speed of 5000ft/s)

Computed results were in close agreement with expectations:

Confined Fluid Test

Computed	Expected
f=1.0	1.0
T=300.9	301.0
p=6.907e+6	6.977e6
ρ=0.9997	1.0

In this test the pressure increases to compensate for the inability of the flow to expand.

Unconfined Fluid Test

Computed	Expected	
f=1.0	1.0	
f_s=0.003	0.003	(expansion into surface cell)
T=301.0	301.0	
p≅9e-6	0.0	
ρ=0.9997	0.9997	

Having a free surface the flow is able to expand (i.e., f_s>0 in the surface cell) and the pressure remains close to zero.

Input file for test problems (version 10.0 of ***FLOW-3D***)

```
Test of Thermal Expansion - 1D Confined

 $xput
    remark='units are cgs',
```

```
   twfin=1.0,
   itb=1,
   dtmax=0.01,
   ifenrg=2,
   igmres=2,
   iadix=0,
   iadiy=0,
   iadiz=1,
   ifdynconv=1,
   epsadj=0.01,
   ifrho=1,
   ifthexp=1,
   iqsr=0,
   ithrmst=0,
$end

$limits
$end

$props
   rcsql=4.3e-11, remark='nominal sound speed 5000ft/s',
   tunits='u',
   mu1=0.01,
   thexf1=0.0003,
   cv1=4.187e7,
   pofl1=4.187e7, remark='source raises T 1deg/s',
   tstar=300.0,
   rhof=1.0,
   thc1=6.5e4,
$end

$scalar
$end

&PCAP
/

$bcdata
   remark='!! Boundary condition Z Min',
   ibct(5)=2,

   remark='!! Boundary condition Z Max',
   ibct(6)=2,

   remark='!! Boundary condition common parameters',
   timbct(1)=0.0,
$end

$mesh
   nxcelt=1,
   px(1)=0,
   px(2)=1.0,

   nycelt=1,
   py(1)=0,
   py(2)=1.0,
```

```
    nzcelt=10,
    pz(1)=0,
    pz(2)=10.0, remark='confined fluid',
 $end
    nzcelt=12, pz(2)=12.0, remark='unconfined fluid',

 $obs
 $end

 $fl
    pvoid=0.0,
    presi=0.0,
    flht=10.0,
    iflinittyp=1,
 $end

 $bf
 $end

 $temp
    tempi=300.0,
 $end

 $motn
 $end

 $grafic
 $end

 &header
    project='TN58_CONFINED',
 /

 $parts
 $end
Documentation: Pressure should increase by 6.977e6 for 1 deg increase
in temperature in confined flow situations.

#start tables:

#fluid1:
#end fluid1

#fluid2:
#end fluid2
#end start tables
```