technical briefs

# Approximation of Fundamental Equations for Finite-Dimensional Modeling of Thermo-Fluid Processes

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## Nomenclature

$A$ = area
$C_p$ = specific heat at constant pressure
$C_v$ = specific heat at constant volume
$cs$ = control surface
$cv$ = control volume
$e$ = sum of specific internal energy, kinetic energy and potential energy
$g$ = acceleration due to gravity
$h$ = specific enthalpy
$n$ = unit normal vector
$p$ = pressure
$Q$ = transferable heat
$T$ = absolute temperature
$t$ = time
$u$ = specific internal energy
$V$ = volume
$v$ = velocity
$W$ = shaft work
$z$ = gravitational head
$1$ = subscript for inlet conditions
$2$ = subscript for exit conditions
$\alpha$ = coefficient of thermal expansion $[-(1/\rho)(\partial\rho/\partial T)_p]$
$\beta$ = isothermal compressibility $[(1/\rho)(\partial\rho/\partial p)_T]$
$\delta$ = arbitrary parameter
$\epsilon$ = arbitrary parameter
$\phi_h$ = partial derivative $(\partial p/\partial h)_\rho$
$\phi_\rho$ = partial derivative $(\partial p/\partial \rho)_h$
$\rho$ = density

*Finite-dimensional lumped models of thermo-fluid processes are usually formulated from fundamental conservation equations. In dynamic modeling and system simulation, internal energy is often replaced by enthalpy in the energy conservation equation without considering the work term $(p/\rho)$. For compressible fluids, this leads to a significant dynamic error, although the steady-state results are unchanged. A more exact formulation, presented here, can be easily implemented. A numerical example is given for a typical case.*

## Introduction

In many industrial systems, modeling and simulation of thermo-fluid processes are essential for dynamic analysis and controller design. Generally, these processes are described by nonlinear partial differential equations with space and time as independent variables. The finite difference method is one of the several ways of numerically solving these equations [1–3], in which case, an infinite-dimensional distributed process is approximated by a finite-dimensional lumped model consisting of a set of ordinary differential equations with time as the independent variable. These models can be easily arranged in state-space form for digital simulation and controller design.

Dynamic equations are usually derived from fundamental principles of mass, momentum and energy conservation [4, 5]. In power plant modeling and simulation, there are several instances where internal energy in the energy conservation equation has been replaced by enthalpy without considering the work term $(p/\rho)$ [6–9]. For relatively incompressible fluids, such as subcooled water, this approximation is justified because the relation $C_p - C_v = T\alpha^2/(\beta\rho)$ implies $C_p \approx C_v$ [10]. But for compressible fluids, such as superheated steam, the difference is significant. Transient performance prediction and controller design of power generation systems [7–9, 11] made on the basis of this approximation may yield misleading conclusions. This technical note shows how a significant dynamic error can result.

A more exact representation can be easily implemented for dynamic modeling and simulation. A numerical example is given for quantitative estimation of dynamic error in the case of steam at throttle conditions typical of a large generating unit.

## Analysis

The fundamental equations for mass and energy conservation in integral form (using Cartesian tensor notation) [4, 5] are

$$0 = \frac{\partial}{\partial t}\int\int_{cv}\int \rho dV + \int_{cs}\int \rho v_i n_i dA \tag{1}$$

$$\dot{Q} - \dot{W} = \frac{\partial}{\partial t}\int\int_{cv}\int e\rho dV + \int_{cs}\int \left(e + \frac{p}{\rho}\right)\rho v_i n_i dA \tag{2}$$

where $\dot{Q} = \bar{d}Q/dt$, $\dot{W} = \bar{d}W/dt$, and operator $\bar{d}$ signifies an inexact differential [10].

Kinetic and gravitational energies are usually small compared to internal energy. Therefore,

$$e = u + \frac{v^2}{2} + gz \simeq u \tag{3}$$

Assuming uniform flow over any cross-section (i.e., one-dimensional flow field) and using a lumped parameter approximation, equations (1), (2), and (3) yield

$$\frac{d}{dt}(\rho V) = \rho_1 v_1 A_1 - \rho_2 v_2 A_2 = F_1 - F_2 \tag{4}$$

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$$\frac{d}{dt}(u\rho V) = \rho_1 v_1 A_1 h_1 - \rho_2 v_2 A_2 h_2 + \dot{Q} - \dot{W}$$

$$= F_1 h_1 - F_2 h_2 + \dot{Q} - \dot{W} \tag{5}$$

where $u$ and $\rho$ are averaged over the entire control volume. Equation (5) is truly satisfied only in infinitesimally small control volumes for thermodynamically simple substances [4, 10]. It is assumed to be an approximation to the present conditions of averaging within the entire control volume. For a fixed control volume and no shaft work,

$$\frac{d\rho}{dt} = (F_1 - F_2)/V \tag{6}$$

$$\frac{d}{dt}(u\rho) = (F_1 h_1 - F_2 h_2 + \dot{Q})/V \tag{7}$$

In some earlier publications [6–9], $u$ in the dynamic term is simply replaced by $h$ and equation (7) is expressed as

$$\frac{d}{dt}(h\rho) = (F_1 h_1 - F_2 h_2 + \dot{Q})/V \tag{7a}$$

Henceforth, all equations with suffix "$a$" follow equation (7a). The purpose of this note is to illustrate the differences between the results obtained from equations (7) and (7a).

Taking time derivatives of both sides in the thermodynamic state equation relating $h$, $u$ and $\rho$,

$$\frac{d}{dt}(h\rho) = \frac{d}{dt}(u\rho) + \frac{dp}{dt}$$

$$= \frac{d}{dt}(u\rho) + \phi_h \frac{dh}{dt} + \phi_\rho \frac{d\rho}{dt} \tag{8}$$

where $\phi_h \triangleq (\partial p/\partial h)_\rho$ and $\phi_\rho \triangleq (\partial p/\partial \rho)_h$.

Substituting equation (8) in equation (7) yields

$$\frac{d(h\rho)}{dt} = [F_1 h_1 - F_2 h_2 + \dot{Q}]/V + \phi_h \frac{dh}{dt} + \phi_\rho \frac{d\rho}{dt}$$

which is rearranged with equation (6) as

$$\frac{dh}{dt} = [F_1(h_1 - h) - F_2(h_2 - h) + (F_1 - F_2)\,\phi_\rho + \dot{Q}]/[V(\rho - \phi_h)] \tag{9}$$

On the other hand, substituting equation (6) in equation (7a) yields

$$\frac{dh}{dt} = [F_1(h_1 - h) - F_2(h_2 - h) + \dot{Q}]/(V\rho) \tag{9a}$$

Equations (9) and (9a) yield the same steady-state results because $F_1 = F_2$ from equation (6).

## Numerical Example

To estimate the difference between equations (9) and (9a), consider an adiabatic and thermodynamically homogeneous control volume (i.e., $\dot{Q} = 0$, $h_2 = h$ and $\rho_2 = \rho$) at typical throttle steam conditions:

$p = 1.6651 \times 10^7$ N/m$^2$ (2415 psia) and $T = 510$°C (950°F)

$h = 3.3168 \times 10^6$ J/kg (1426.4 Btu/lbm)

and $\rho = 53.161e + 01$ kg/m$^3$ (3.31 lbm/ft$^3$)

The thermodynamic state relationship in this range is obtained from steam table data [12].

$$p = 6.6576 \times 10^4 + (0.23236h - 4.5873 \times 10^5)\,\rho$$

where $p$, $h$ and $\rho$ are in SI units.

The partial derivatives are

$$\phi_h = \left(\frac{\partial p}{\partial h}\right)_\rho = 0.23236\rho = 12.353 \text{ kg/m}^3$$

$$\phi_\rho = \left(\frac{\partial p}{\partial \rho}\right)_h = 2.23236h - 4.5873 \times 10^5 = 3.1196 \times 10^5 \text{ J/kg}$$

At steady state, equations (6) and (9) or (9a) yield

$$F_1 = F_2 \text{ and } h_1 = h$$

Consider small step disturbances in $F_1$ and $h_1$ of $\delta$ per unit and $\epsilon$ per unit, respectively, from the initial steady state. Thus at the instant $t = 0^+$, $F_1 = (1 + \delta)F_2$ and $h_1 = (1 + \epsilon)h$; and then $dp/dt = \phi_\rho\, d\rho/dt + \phi_h\, dh/dt$ is evaluated from equations (6), (9) and (9a) as

$$D \triangleq \frac{dp}{dt} = [\delta\rho\phi_\rho + (1 + \delta)\epsilon h \phi_h]\frac{F_2}{V} \Big/ (\rho - \phi_h) \tag{10}$$

in the present case and

$$D_a \triangleq \frac{dp}{dt} = [\delta\rho\phi_\rho + (1 + \delta)\epsilon h \phi_h]\frac{F_2}{V} \Big/ \rho \tag{10a}$$

in some earlier cases.

The relative error $(1 - D_a/D)$ in the initial value of $dp/dt$ is evaluated as $1 - D_a/D = \phi_h/\rho = 0.2323$, that is the relative error is approximately 23 percent.

## Conclusions

A significant dynamic error is introduced by replacing the internal energy term in the energy conservation equation by enthalpy without considering the work term $(p/\rho)$—a frequent approximation in modeling and simulation of power generation systems. Transient performance prediction and controller design made on the basis of such models may yield misleading conclusions.

A more exact derivation, obtained from a lumped representation of the mass and energy conservation equations, can be easily implemented in dynamic modeling and simulation. A numerical example for a typical case indicates an error at 23 percent.

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