
PROCESS DYNAMIC SIMULATION

An Introduction To The Fundamental Equations

First Edition

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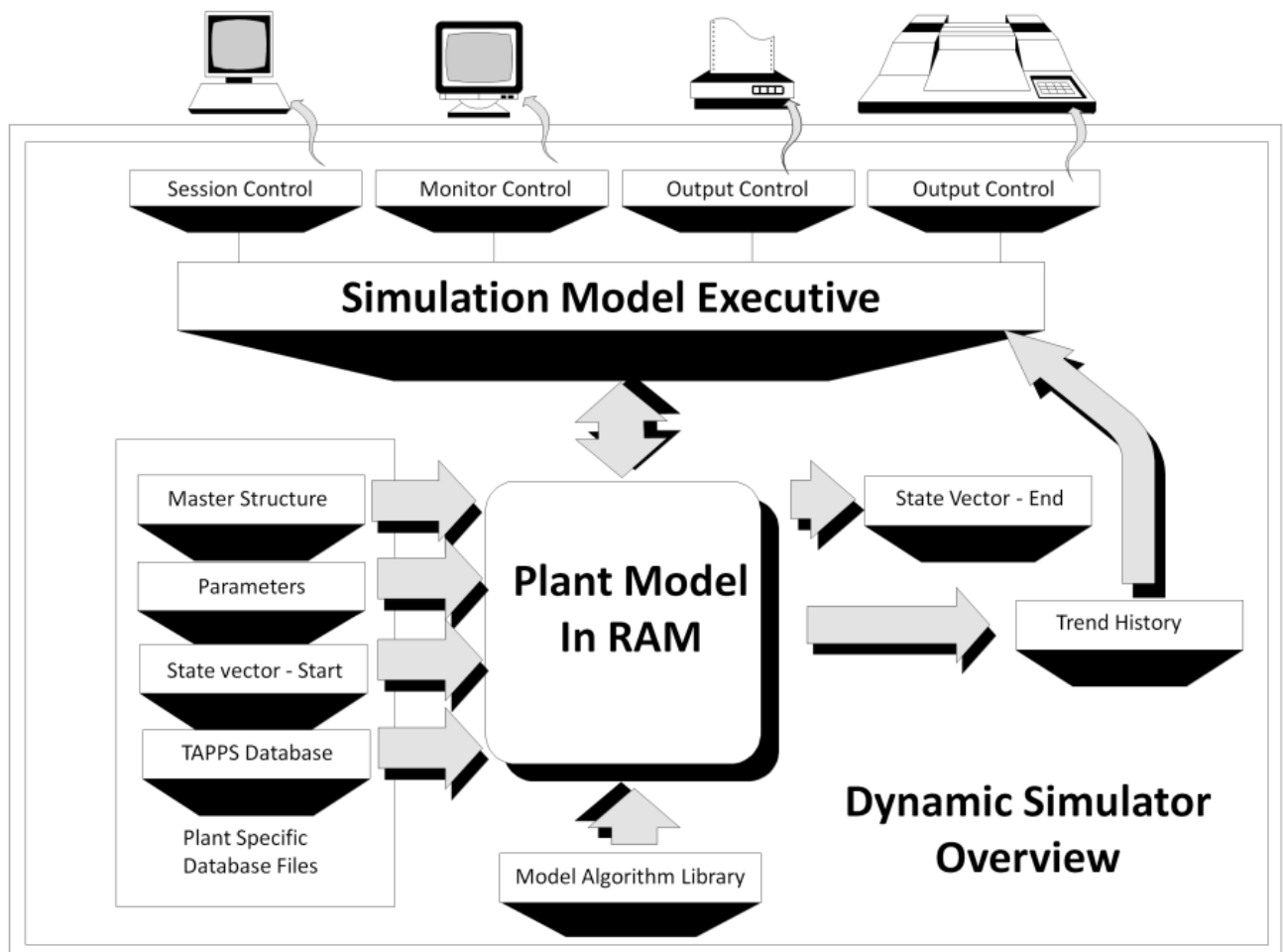
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PREFACE

The rapid increase of computing power at affordable prices during the past few years, together with advances in process modelling and simulation technology, has enabled *dynamic process simulation* to become an established tool in the Process Industry for *problem solving* and *control strategy verification*. In fact, it is hard to visualise a situation where some critical processes could be implemented without a dynamic simulation having previously been performed to verify the viability of the control system. The situation has now been reached where these improvements make it possible to produce very accurate *simulated* full-scale process pilot-plants.

Dynamic process simulation differs from purely steady-state simulation in that the former requires the mechanical construction of process items be taken into account; the amount of mechanical detail being dependant upon the particular application. The reason for this is that *dynamic mass, energy and momentum balances* have to be continuously updated. These calculations are fundamental to dynamic process simulation and they require knowledge of volumes, metal mass, etc., to predict the proper dynamic behaviour of a particular plant. My intention in writing this technical bulletin was to produce a short document that would provide some insight in to the physical basis for the fundamental mass and energy balance equations used in process dynamic simulation, and how they are derived. For each accumulation process considered, I have first defined the appropriate macroscopic integral and differential equations and, when appropriate, followed these by derivations of the partial differential equations which describe the associated microscopic system. For practical problems, solutions are obtained by numerical integration of these equations w.r.t. time - analytical solutions are rarely possible due to the highly non-linear nature of chemical processes. The equations detailed in this bulletin, together with rigorous thermodynamic and physical property predictions, form the basis of process models used in the AspenTech® dynamic process simulators.

It is only by paying great attention to detail that process models can be made sufficiently accurate to reflect the operational behaviour of a real plant; this applies particularly to dynamic process models. The best test of model accuracy is comparison with real plant behaviour over wide operating regimens. AspenTech® models have consistently met the highest standards as demanded by the Industry, and provided accurate predictions of dynamic behaviour for wide-ranging applications. The international recognition of our success in achieving this aim is very pleasing to us, though we are not complacent. We have an ongoing development programme and are constantly striving to improve our service and to achieve higher and higher fidelity models. However, the quality we have obtained is not due solely to the sophistication of the mathematics utilised within our models, it is due in equal part to the high level of engineering content inherent in them. This results from continuous feedback provided by a team of professionals who use AspenTech® dynamic simulators daily for carrying out demanding dynamic simulation projects.

The bibliography included as Appendix F provides a list of source material for those people who may wish to take the subject further. Except where stated to the contrary, Cartesian co-ordinates and SI units have been used throughout.

Graham W Griffiths
London
December 1992

LIST OF SYMBOLS

$\hat{\mathbf{a}}$	= unit vector collinear with velocity vector \mathbf{V} (units)
\mathbf{a}	= fluid particle acceleration vector (m/s^2)
\mathbf{A}	= vector function continuous on \mathcal{S} (units)
C_p	= specific heat ($\text{kJ/kg}^\circ\text{K}$)
D	= pipeline diameter (m)
D	= mass diffusivity ($\text{kg/m}^2/\text{s}$)
D^i	= mass diffusivity of i th component (m^2/s)
f	= Moody friction factor (units)
\mathbf{F}	= force vector (N/m^2)
\mathbf{g}	= acceleration vector, due to gravity (9.80665 m/s^2)
h	= specific enthalpy (J/kg)
Δh	= enthalpy drop from inlet to outlet (J/kg)
ΔH_i°	= heat of i th reaction ($\text{J/m}^3/\text{s}$)
I	= moment of inertia (kg m^2)
\mathbf{j}	= mass flux vector ($\text{kg/m}^2/\text{s}$)
J	= mass flow due to diffusion (kg/s)
J^i	= mass flow of i th component due to <i>Diffusion</i> (kg/s)
k	= thermal conductivity of solid ($\text{W/m}^\circ\text{K}$)
K	= specific kinetic energy (J/kg)
L	= pipeline length (m)
\mathbf{L}	= angular momentum ($\text{kg m}^2/\text{s}$)
m	= mass (kg)
m	= mass accumulation (kg)
m^i	= mass accumulation of i th component (kg)
$\hat{\mathbf{n}}$	= unit vector normal to \mathbf{r} and $\boldsymbol{\theta}$
n	= polytropic exponent (units)
MW	= molecular weight (units)
N	= revolutions per second ($1/\text{s}$)
p	= pressure (Pa)
p_{g1}	= inlet gas pressure (Pa)
p_{g2}	= outlet gas pressure (Pa)
P_D	= power delivered to the shaft by driver (W , J/s)
P_L	= power absorbed by load (W , J/s)
\mathbf{P}	= linear momentum (kg m/s)
\mathbf{q}	= heat flux vector ($\text{J/m}^2/\text{s}$).
Q	= heat transfer rate (J/s)
$\hat{\mathbf{r}}$	= unit position vector, etc., refer to Figure 5.1 (units)
\mathbf{r}	= position vector of mass m (m)
r^i	= rate of mass production or depletion per unit volume of i th component due to <i>Homogeneous Reaction</i> ($\text{kg/m}^3/\text{s}$)

R^i	= rate of mass production or depletion of <i>ith</i> component due to <i>Homogeneous Reaction</i> (kg/s)
R	= ideal gas constant (8314.3 J/kg-mole-°K)
\mathbf{S}	= surface vector (Area \times outward unit normal vector) (m^2)
S_{wall}	= wall surface area (m^2)
\mathbf{S}_{wall}	= wall surface area vector ($S_{wall} \times$ outward unit normal vector) (m^2)
t	= time (s)
T	= temperature (°K)
T_D	= torque applied to shaft by driver (kg m)
T_L	= torque exerted by load (kg m)
T_I	= inlet gas temperature (°K)
u	= specific internal energy (J/kg)
v	= control volume (m^3)
\mathbf{v}	= mass velocity vector (m/s)
V	= volume of gas (m^3)
\mathbf{V}	= fluid velocity vector (m/s)
\mathbf{V}^i	= fluid velocity vector of <i>ith</i> species (m/s)
w	= mass flow due to convection (kg/s)
w^i	= mass flow of <i>ith</i> component (kg/s)
W_g	= mass flow of gas being compressed (kg/s)
W_s	= mass flow of steam (kg/s)
W	= work (J/s)
x,y,z	= spacial co-ordinates in the cartesian system (m)
Z_{ave}	= average of inlet and outlet compressibility (units)

Greek Symbols

α	= thermal diffusivity (m^2/s)
η_c	= efficiency of compressor (units)
η_t	= efficiency of turbine (units)
θ	= angle between gravitational force and velocity vector (radians).
Θ	= angular displacement of position vector (radians)
μ	= viscosity (Ns/m^2).
ρ	= mass density (kg/m^3)
ρ^i	= mass density of <i>ith</i> component (kg/m^3)
τ_w	= stress at pipe wall (Pa)
ϕ	= specific potential energy (J/kg)
ω	= angular speed (radians/s)

Operators

$\nabla \cdot \mathbf{A}$	= divergence of vector \mathbf{A}
∇T	= gradient of scalar T
D/Dt	= substantive derivative, refer to Appendix B

INTRODUCTION

1

Process simulation can be defined as:

"Any calculation or set of calculations carried out in order to predict how a Process Plant or part of a Process Plant will perform under a certain set of circumstances".

Thus, a procedure for calculating the surface area of a heat exchanger would not be classed as process simulation; however, once sized, any subsequent calculation to predict the exchanger's performance under a specified set of conditions, would be considered a process simulation. It is of course realised that other valid definitions are possible.

Dynamic process simulation is used to study the performance of time-dependant processes. It is becoming an increasingly more important main-stream engineering tool that is being used to analyse and design the more complex plants being built today. In particular, it is being called upon to investigate the dynamics and control of highly integrated multi-process plants which often require more difficult control problems to be being tackled than is the case for single plants. It is also becoming essential to use dynamic simulation during the design phase of a project because operational requirements, which are having a greater and greater impact on process design, can only be resolved by this method.

The theoretical basis for dynamic process simulation has been established for many years, and it has been the lack of low cost, powerful computing that has slowed its application. This lack of computing also inhibited the development of good, appropriate software which, thankfully is now being redressed. Proprietary developments in numerical methods and data handling have enabled robust fast integrators to be incorporated into the AspenTech® dynamic simulators. These have provided great improvements in computational speed and have enabled very large scale simulations to be handled, including those with complicated discontinuities.

For maximum benefit, the dynamic simulation should be carried out as early as possible in the life of a project. This is to avoid engineers proceeding with the detailed design of a plant which may subsequently require changes to be made as a result of deficiencies exposed by simulation. It also means that a simulation model can follow a project through its life cycle providing a valuable source of information along the way.

Dynamic simulation is an activity that inherently involves the solution of differential equations having time as the independent variable. For dynamic process simulation these differential equations generally represent accumulation of *mass*, *energy* and *momentum* in one form or another. It is the rate-of-change of these fundamental physical quantities that actually determines the intrinsic dynamic behaviour of a chemical process, and to solve the associated equations involves a significant amount mathematics. The overall dynamic behaviour of a process plant is also dependant upon the performance of actuators and their control systems.

Dynamic process simulation differs from purely steady-state simulation in that the former requires the mechanical construction of process items be taken into account; the amount of mechanical detail being dependant upon the particular application. The reason for this is that the dynamic mass, energy and momentum balances have to be continuously updated. These calculations are fundamental to dynamic process simulation and they require knowledge of volumes, metal mass, etc., to predict the proper dynamic behaviour of a particular plant.

This technical bulletin has been prepared in order to provide some insight into the physical basis for the fundamental mass, energy and momentum balance equations used in process dynamic simulation, and how they are derived. It is aimed at graduate chemical, mechanical and control engineers who are interested in familiarising themselves with the physical basis for dynamic process simulation and, for this reason, the analysis of control systems and other associated topics have been excluded. For each accumulation process considered, the appropriate macroscopic integral and differential equations are defined and, when appropriate, these are followed by derivations of the partial differential equations which describe the associated microscopic system. For practical problems, solutions are obtained by numerical integration of these equations w.r.t. time - analytical solutions are rarely possible due to the highly non-linear nature of chemical processes. The equations detailed in this bulletin, together with rigorous thermodynamic and physical property predictions, form the basis of process models used in the AspenTech ® dynamic process simulators.

Finally, it is appropriate to emphasise that only by paying great attention to detail is it possible to make process models that are sufficiently accurate to reflect the operational behaviour of a real plant; this applies particularly to dynamic process models. The best test of model accuracy is comparison with real plant behaviour over wide operating regimens. AspenTech ® models have consistently met the highest standards as demanded by the Industry, and provided accurate predictions of dynamic behaviour for wide-ranging applications.

THE DYNAMIC MASS BALANCE

2
2.1 MACROSCOPIC SYSTEM

If we consider a control volume with mass flowing in and out, then the dynamic mass balance can be described as follows:

$$\{\text{Rate of change of Mass accumulation}\} = \Sigma\{\text{Mass flows in}\} - \Sigma\{\text{Mass flows out}\}$$

Which can be represented mathematically as,

$$\frac{\partial}{\partial t} \iiint_{\nu} \rho \, dv = \iint_{\mathcal{S}} \rho \mathbf{V} \cdot d\mathbf{S} - \iint_{\mathcal{S}} \mathbf{j} \cdot d\mathbf{S} \quad (1)$$

where,

ρ = mass density (kg/m³)

\mathbf{j} = mass flux vector (kg/m²/s)

ν = control volume (m³)

\mathbf{V} = fluid velocity vector (m/s)

\mathbf{S} = surface vector (Area \times outward unit normal vector) (m²)

The first term on the R.H.S. of the above equation represents mass flow due to *Convection* and the second term represents mass flow due to *Diffusion*.

For a *macroscopic system* containing a *well mixed homogeneous* fluid with a known boundary, equation (1) can be integrated to give,

$$\frac{d(\rho\nu)}{dt} = (\rho_{in} \mathbf{V}_{in} \cdot \mathbf{S}_{in} - \rho_{out} \mathbf{V}_{out} \cdot \mathbf{S}_{out}) + (\mathbf{j}_{in} \cdot \mathbf{S}_{in} - \mathbf{j}_{out} \cdot \mathbf{S}_{out}) \quad (2)$$

If the surface vector \mathbf{S} is collinear with the velocity vector \mathbf{V} and mass flux vector \mathbf{j} , then the dot products become equal to products of the associated vector magnitudes. Under these circumstances, equation (2) becomes,

$$\frac{d(\rho v)}{dt} = (\rho_{in} V_{in} S_{in} - \rho_{out} V_{out} S_{out}) + (J_{in} S_{in} - J_{out} S_{out}) \quad (3)$$

For a system with multiple flows in and out equation (3) can be rewritten in engineering units to give a suitable working equation, i.e.

$$\frac{dm}{dt} = \sum w_{in} - \sum w_{out} + J_{in} - J_{out} \quad (4)$$

Where,

- J = mass flow due to diffusion (kg/s)
- m = mass accumulation (kg)
- w = mass flow due to convection (kg/s)

Equation (4) represents the macroscopic *Continuity* or, *Total Mass Balance* equation, and is used for calculations involving systems comprising holdups that can be assumed to contain homogeneous well mixed fluids.

For a dynamic simulation, equation (4) would be integrated w.r.t. time using numerical techniques, either for a fixed period or continuously, depending upon the application.

2.2 MACROSCOPIC SYSTEM - Multicomponent

When a multicomponent fluid is under consideration then, in addition to the mass balance equation (4), mass balance equations are needed for each species, i.e.

$$\frac{dm^i}{dt} = \sum w_{in}^i - \sum w_{out}^i + J_{in}^i - J_{out}^i + R^i \quad (5)$$

Where,

- m^i = mass accumulation of *ith* component (kg)
- J^i = mass flow of *ith* component due to *Diffusion* (kg/s)
- R^i = rate of mass production or depletion of *ith* component due to *Homogeneous Reaction* (kg/s)
- w^i = mass flow of *ith* component (kg/s)

The derivation of equation (5) is carried out in a similar way to that used in section 2.1. R^i is obtained from an appropriate *Reaction Kinetic Equation* and J^i is obtained from the *Diffusion Equation*.

2.3 MICROSCOPIC SYSTEM

The R.H.S. of equation (1) can be transformed by use of the Divergence Theorem (see Appendix A), i.e.

$$-\iint_S \rho \mathbf{V} \cdot d\mathbf{S} - \iint_S \mathbf{j} \cdot d\mathbf{S} = -\iiint_V \nabla \cdot (\rho \mathbf{V}) dv - \iiint_V \nabla \cdot \mathbf{j} dv \quad (6)$$

Thus, equation (1) can be rewritten as,

$$\frac{\partial}{\partial t} \iiint_V \rho dv = -\iiint_V \nabla \cdot (\rho \mathbf{V}) dv - \iiint_V \nabla \cdot \mathbf{j} dv \quad (7)$$

For a stationary volume the time differential can be included under the integral sign,

$$\therefore \iiint_V \frac{\partial \rho}{\partial t} dv = -\iiint_V \nabla \cdot (\rho \mathbf{V}) dv - \iiint_V \nabla \cdot \mathbf{j} dv \quad (8)$$

On rearranging, equation (8) simplifies to,

$$\iiint_V \left\{ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) + \nabla \cdot \mathbf{j} \right\} dv = 0 \quad (9)$$

Since the limits of integration are arbitrary, the quantity inside the brackets must be equal to zero. Also, the third term inside the brackets can be expanded by use of Fick's law of diffusion, i.e.

$$\mathbf{j} = -D \nabla \rho \quad (10)$$

where,

D = mass diffusivity (kg/m²/s)

Thus,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{V}) + D \nabla^2 \rho \quad (11)$$

Equation (11) represents the microscopic *Continuity* or, *Total Mass Balance* equation. For a unidimensional system subject only to axial variations in the z direction, such as a pipeline where radial effects are not considered, equation (11) becomes,

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho V_z)}{\partial z} + D_z \frac{\partial^2 \rho}{\partial z^2} \quad (12)$$

For applications with significant convection flow, the diffusion term in the above equation can often be neglected.

For a dynamic simulation, equation (12) is usually solved using numerical techniques such as:

- o finite difference,
- o finite element,
- o orthogonal collocation.

It is sometimes convenient to group together the first derivatives of ρ to form the *substantive derivative*, refer to Appendix B. Thus, if we neglect diffusion and differentiate the term in parenthesis, equation (12) can be rearranged as shown below,

$$\frac{D\rho}{Dt} = -\rho \frac{\partial V_z}{\partial z} \quad (13)$$

or, in vector form,

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{V} \quad (14)$$

Equation (14) represents the equation of *Continuity* for an observer following the fluid at the same velocity. In this situation D/Dt represents the *substantive derivative* operator.

2.4 MICROSCOPIC SYSTEM - Multicomponent

When a multicomponent fluid is under consideration then, in addition to the *Continuity* equation (11), a mass balance equation is needed for each species, i.e.

$$\therefore \frac{\partial \rho^i}{\partial t} = -\nabla \cdot (\rho^i \mathbf{V}^i) + D^i \nabla^2 \rho^i + r^i \quad (15)$$

where,

ρ^i = mass density of *ith* component (kg/m³)

D^i = mass diffusivity of *ith* component (m²/s)

r^i = rate of mass production or depletion per unit volume of *ith* component due to
Homogeneous Reaction (kg/m³/s)

\mathbf{V}^i = velocity of *ith* species (m/s)

Derivation of the above equation is carried out in a similar way to that used in section 2.2. With regard to the R.H.S. of equation (15), the first and second terms represent mass transport of the *ith* component due to *Convection* and *Diffusion* respectively, whilst the third term represents generation due to *Reaction*.

THE DYNAMIC ENERGY BALANCE - Total

3
3.1 MACROSCOPIC SYSTEM

If we consider a control volume with mass flowing in and out, then the dynamic energy balance can be described as follows:

$$\{\text{Rate of change of Energy accumulation}\} = \Sigma\{\text{Energy flows in}\} - \Sigma\{\text{Energy flows out}\}$$

Which can be represented mathematically as,

$$\frac{\partial}{\partial t} \iiint_V (u + \phi + K) \rho dv + \iint_S (h + \phi + K) \rho \mathbf{V} \cdot d\mathbf{S} = Q - W + \iiint_V \Sigma \Delta H_i^{\circ} dv \quad (16)$$

where,

- u = specific internal energy (J/kg)
- h = specific enthalpy (J/kg)
- ϕ = specific potential energy (J/kg)
- K = specific kinetic energy (J/kg)
- ρ = mass density (kg/m^3)
- Q = heat transfer (J/s)
- W = work (J/s)
- p = pressure (Pa)
- ΔH_i° = heat of *ith* reaction ($\text{J/m}^3/\text{s}$)

and,

$$h = u + \frac{p}{\rho} \quad (17)$$

For a macroscopic system containing a well-mixed fluid with a known boundary, and where potential and kinetic energy effects are minimal, equation (16) can be integrated to give,

$$\frac{d(\rho v u)}{dt} = \rho_{in} h_{in} \mathbf{V}_{in} \cdot \mathbf{S}_{in} - \rho_{out} h_{out} \mathbf{V}_{out} \cdot \mathbf{S}_{out} + Q - W + v \sum \Delta H_i^o \quad (18)$$

If the surface vector \mathbf{S} is collinear with the velocity vector \mathbf{V} , then the dot products become equal to products of the associated vector magnitudes. Under these circumstances, which would apply to say, a holdup vessel with inlet and outlet piping, equation (18) becomes,

$$\frac{d(mu)}{dt} = \sum w_{in} h_{in} - \sum w_{out} h_{out} + Q - W + v \sum \Delta H_i^o \quad (19)$$

Neglecting potential and kinetic energy effects is usually justifiable in most practical situations involving process plant vessels. However, should it be necessary to include for these effects, then they are easily accounted for in the same way as for the enthalpy flows in and out.

Equation (19) represents the macroscopic *Total Energy Balance* equation, and is used for calculations involving systems comprising holdups that can be assumed to contain homogeneous well mixed fluids.

For a dynamic simulation, equation (19) would be integrated w.r.t. time using numerical techniques.

3.2 MICROSCOPIC SYSTEM

Using equation (17), the second term on the left-hand side of equation (16) becomes,

$$\iint_S (h + \phi + K) \rho \mathbf{V} \cdot d\mathbf{S} = \iint_S \{ (u + \phi + K) \rho + p \} \mathbf{V} \cdot d\mathbf{S} \quad (20)$$

Let,

$$\Omega = (u + \phi + K) \quad (21)$$

Then, after applying the Divergence Theorem to equation (16) and rearranging, we obtain,

$$\iiint_v \left\{ \frac{\partial \rho \Omega}{\partial t} + (\rho \Omega + p) \nabla \cdot \mathbf{V} - \sum \nabla H_i^o \right\} dv = Q - W \quad (22)$$

If we consider Q to be the rate of heat transfer to the control volume v expressed in terms of heat flux, then

$$Q = \iint_S \mathbf{q} \cdot d\mathbf{S} \quad (23)$$

where,

\mathbf{q} = heat flux vector (J/m²/s).

By use of the Divergence Theorem we obtain,

$$\iint_S \mathbf{q} \cdot d\mathbf{S} = \iiint_v \nabla \cdot \mathbf{q} \, dv \quad (24)$$

If we also consider W to be the rate of surface work done on the control volume, then

$$W = \iint_S [\mathbf{T} \cdot \mathbf{V}] \cdot d\mathbf{S} \quad (25)$$

where,

$$\mathbf{T} = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} \quad (26)$$

is the stress tensor, where the individual elements have units of pressure (Pa).

For Newtonian fluids, i.e. those that obey Newton's law of viscosity,

$$\tau_{xy} = \mu \frac{dV_x}{dy}, \dots, etc \quad (27)$$

where,

μ = viscosity (Ns/m²),

the Divergence Theorem gives,

$$\iint_S [\mathbf{T} \cdot \mathbf{V}] d\mathbf{S} = \iiint_V \nabla \cdot [\mathbf{T} \cdot \mathbf{V}] dv \quad (28)$$

Using the results of equations (24) and (28), and rearranging equation (22) gives,

$$\iiint_V \left\{ \frac{\partial \rho \Omega}{\partial t} + (\rho \Omega + p) \nabla \cdot \mathbf{V} - \sum \nabla H_i^o - \nabla \cdot \mathbf{q} + \nabla \cdot [\mathbf{T} \cdot \mathbf{V}] \right\} dv = 0 \quad (29)$$

Again, since the limits of integration are arbitrary, the quantity inside the brackets must be equal to zero.

$$\therefore \frac{\partial \rho \Omega}{\partial t} + (\rho \Omega + p) \nabla \cdot \mathbf{V} - \sum \nabla H_i^o - \nabla \cdot \mathbf{q} + \nabla \cdot [\mathbf{T} \cdot \mathbf{V}] = 0 \quad (30)$$

Equation (30) represents the *Differential Total Energy Balance* equation.

THE DYNAMIC MOMENTUM BALANCE

4

4.1 MACROSCOPIC SYSTEM

If we consider a control volume with mass flowing in and out, then the dynamic momentum balance can be described as follows:

$$\{ \text{Net Force} \} = \{ \text{Momentum flow in} \} - \{ \text{Momentum flow out} \} + \{ \text{Rate of change of Momentum accumulation} \}$$

Which, neglecting diffusion effects, can be represented mathematically as,

$$\Sigma \mathbf{F} = \iint_S \mathbf{V}(\rho \mathbf{V} \cdot d\mathbf{S}) + \frac{\partial}{\partial t} \iiint_V \rho \mathbf{V} \, dv \quad (31)$$

The expression in parentheses of the first term on the R.H.S. of equation (31) represents mass flow across the surface $d\mathbf{S}$; thus, multiplying this mass by \mathbf{V} gives the corresponding momentum flow. The parentheses also imply that the dot product must be performed prior to multiplying by \mathbf{V} .

The net force consists of three components which arise due to the effects of: 'gravity', 'pressure' and 'viscous friction', i.e.

$$\Sigma \mathbf{F} = \mathbf{F}_g + \mathbf{F}_p + \mathbf{F}_f \quad (32)$$

The force due to *gravity* is defined by,

$$\mathbf{F}_g = \iiint_V \rho \mathbf{g} \, dv \quad (33)$$

where,

\mathbf{g} = acceleration vector, due to gravity (9.80665 m/s²)
 \mathbf{F} = force vector (N/m²)

The force due to *pressure* is defined by,

$$\mathbf{F}_P = \iint_S p d\mathbf{S} \quad (34)$$

The force due to *viscous friction* is defined by,

$$\mathbf{F}_f = \iint_S [\mathbf{T}] \cdot d\mathbf{S} \quad (35)$$

For a *macroscopic system* containing a well mixed homogeneous fluid with known boundary, we can substitute equations (33), (34) and (35) into equation (31) and integrate to give,

$$\frac{d(\rho v \mathbf{V})}{dt} = \mathbf{V}_{in} (\rho_{in} \mathbf{V}_{in} \cdot \mathbf{S}_{in}) - \mathbf{V}_{out} (\rho_{out} \mathbf{V}_{out} \cdot \mathbf{S}_{out}) - \rho v \mathbf{g} + p_{in} \mathbf{S}_{in} - p_{out} \mathbf{S}_{out} - [\mathbf{T}] \cdot \mathbf{S}_{wall} \quad (36)$$

The surface integrals have been evaluated over the entire system surface, though only part of the surface contributes to the momentum balance. Equation (36) represents a system such as a pipeline, where the appropriate contributing surfaces are indicated. The last term represents a complex tensor relationship that can be simplified if we assume that all viscous friction losses take place at the system surface. Under these conditions the viscous term results in a vector collinear with velocity vector \mathbf{V} , having magnitude equal to the product of stress and system wall surface area, i.e.

$$\frac{d(\rho v \mathbf{V})}{dt} = \mathbf{V}_{in} \rho_{in} \mathbf{V}_{in} \cdot \mathbf{S}_{in} - \mathbf{V}_{out} \rho_{out} \mathbf{V}_{out} \cdot \mathbf{S}_{out} - \rho v \mathbf{g} + p_{in} \mathbf{S}_{in} - p_{out} \mathbf{S}_{out} - \tau_w S_{wall} \hat{\mathbf{a}} \quad (37)$$

Where,

- $\hat{\mathbf{a}}$ = unit vector collinear with velocity vector V (units)
- S_{wall} = wall surface area (m^2)
- \mathbf{S}_{wall} = wall surface area vector ($S_{wall} \times$ outward unit normal vector) (m^2)
- τ_w = stress at pipe wall (Pa)

Before we can simplify equation (37) further, it is necessary to find a working relationship for τ_w . For relatively straightforward systems involving pipelines, we can use bulk flow properties and assume that at steady state, forces in the direction of flow are in equilibrium, i.e.

$$\{ \text{Net Pressure Force} \} = \{ \text{Net Sheer Stress Force At Pipe Wall} \}.$$

The above can be expressed mathematically as,

$$p_{in} \mathbf{S}_{in} - p_{out} \mathbf{S}_{out} = \tau_w S_{wall} \hat{\mathbf{a}} \quad (38)$$

or, in scalar form for pipelines having uniform circular cross-section, where inlet and outlet surfaces are normal to

flow,

$$\Delta p \frac{1}{4} \pi D^2 = \tau_w \pi DL \quad (39)$$

Where,

D = pipeline diameter (m)

L = pipeline length (m)

We can now use a form of the fundamental *Darcy* flow equation,

$$\Delta p = \left(\frac{f L}{D} \right) \left(\frac{\rho V^2}{2} \right) \quad (40)$$

to eliminate p from equation (39) to give,

$$\tau_w = \left(\frac{f}{4} \right) \left(\frac{\rho V^2}{2} \right) \quad (41)$$

Where,

f = Moody friction factor (units)

$$\therefore \tau_w S_{wall} = \frac{1}{8} \pi DL f \rho V^2 \quad (42)$$

We now consider a homogeneous system where the surface vectors \mathbf{S}_{in} and \mathbf{S}_{out} are collinear with the velocity vector \mathbf{V} and, the surface vector \mathbf{S}_{wall} is normal to the velocity vector \mathbf{V} with friction losses occurring only at the vessel wall. Then, by dot multiplying through by the unit velocity vector, equation (37) is transformed into a scalar function where all the dot products, except for the gravitational term, become equal to products of the associated vector magnitudes. Under these conditions, which could apply to incompressible flow in a pipeline, equation (37) becomes,

$$\frac{dV}{dt} = \frac{1}{L} (V_{in}^2 - V_{out}^2) - g \cos \theta + \frac{1}{\rho L} (p_{in} - p_{out}) - \frac{f}{2D} V^2 \quad (43)$$

Where,

θ = the angle between the gravitational force and the velocity vector (radians).

For pipelines having uniform cross section the kinetic energy term is zero, therefore equation (43) can be simplified to the following working form,

$$\frac{dV}{dt} = \frac{1}{\rho L} (p_{in} - p_{out}) - \frac{f}{2D} V^2 - g \cos \theta \quad (44)$$

For a dynamic simulation, equation (44) would be integrated using numerical techniques.

4.2 MICROSCOPIC SYSTEM

If we assume a stationary control volume, then on applying the Divergence Theorem to equation (31), we obtain,

$$\Sigma \mathbf{F} = \iiint_V \nabla \cdot \mathbf{V} \rho \mathbf{V} dv + \iiint_V \frac{\partial \rho \mathbf{V}}{\partial t} dv \quad (45)$$

Using equations (33), (34) and (35), equation (45) becomes,

$$\iiint_V \rho \mathbf{g} dv - \iint_S p d\mathbf{S} - \iint_S [\mathbf{T}] \cdot d\mathbf{S} = \iiint_V \nabla \cdot \mathbf{V} \rho \mathbf{V} dv + \iiint_V \frac{\partial \rho \mathbf{V}}{\partial t} dv \quad (46)$$

Applying the Divergence Theorem to equation (46) and rearranging gives,

$$\iiint_V \left\{ \frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \mathbf{V} \rho \mathbf{V} - \rho \mathbf{g} + \Delta p + \nabla \cdot [\mathbf{T}] \right\} dv = 0 \quad (47)$$

Again, since the limits of integration are arbitrary, the quantity inside the brackets must be equal to zero. Thus, on rearranging the second term we obtain,

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \rho \mathbf{V} \mathbf{V} - \rho \mathbf{g} + \Delta p + \nabla \cdot [\mathbf{T}] = 0 \quad (48)$$

Equation (48) represents the *Differential Momentum Balance* equation.

It should be noted that when evaluating equation (48), the second term does **NOT** represent a simple divergence owing to the tensorial nature of $\rho \mathbf{V} \mathbf{V}$, refer to Appendix C. The physical interpretation of the second term is that it represents the rate-of-change of momentum per unit volume by fluid flow. Equation (48) can be simplified using the *Continuity Equation* (equation (11)) to formulate the *Navier-Stokes Equations*, refer to Appendix D.

THE DYNAMIC ENERGY BALANCE - Thermal Conduction

5
5.1 MACROSCOPIC SYSTEM

If we consider a control volume with heat flow in and out, then the dynamic energy balance for a solid can be described as follows:

{Rate of change of Energy accumulation} = Σ {Energy flows in} - Σ {Energy flows out}

Which can be represented mathematically as,

$$\frac{\partial}{\partial t} \iiint_V \rho C_p T \, dv = \iint_S \mathbf{q} \cdot d\mathbf{S} \quad (49)$$

where,

T = temperature ($^{\circ}\text{K}$)

C_p = specific heat ($\text{kJ/kg}^{\circ}\text{K}$)

For a macroscopic system containing a solid with a known boundary, equation (49) can be integrated to give,

$$\frac{d(\rho v C_p T)}{dt} = \mathbf{q}_{in} \cdot \mathbf{S}_{in} - \mathbf{q}_{out} \cdot \mathbf{S}_{out} \quad (50)$$

For a homogeneous solid where the surface vectors \mathbf{S}_{in} and \mathbf{S}_{out} are collinear with heat flux vectors \mathbf{q}_{in} and \mathbf{q}_{out} respectively, then the dot products becomes equal to the products of the associated vector magnitudes, and equation (50) can be written in the working form,

$\frac{dT}{dt} = \frac{I}{m C_P} \{ Q_{in} - Q_{out} \} \quad (51)$

For a dynamic simulation, equation (51) would be integrated w.r.t. time using numerical techniques.

5.2 THE MICROSCOPIC SYSTEM

From the Divergence Theorem and, assuming a stationary solid, equation (49) can be transformed to,

$$\iiint_V \left\{ \frac{\partial}{\partial t} \rho C_p T - \nabla \cdot \mathbf{q} \right\} dv = 0 \quad (52)$$

Again, since the limits of integration are arbitrary, the quantity inside the brackets must be equal to zero.

$$\therefore \frac{\partial}{\partial t} \rho C_p T - \nabla \cdot \mathbf{q} = 0 \quad (53)$$

But, by Fourier's law of heat conduction,

$$\mathbf{q} = k \nabla T \quad (54)$$

where,

k = thermal conductivity of solid (W/m²/°K)

and assuming a homogeneous solid, equation (53) becomes,

$$\rho C_p \frac{\partial T}{\partial t} - k \Delta^2 T = 0 \quad (55)$$

Let,

$$\alpha = \frac{k}{\rho C_p} \quad (56)$$

where,

α = thermal diffusivity (m²/s)

$$\therefore \frac{\partial T}{\partial t} - \alpha \nabla^2 T = 0 \quad (57)$$

Equation (57) represents the *Thermal Diffusion* equation.

THE DYNAMIC ENERGY BALANCE - Rotating Systems

6

6.1 MACROSCOPIC SYSTEM

If we consider a *rotating mechanical system* subject to driver and load torques, then the dynamic energy balance can be described as follows:

$$\{\text{Rate of change of Angular Momentum}\} = \Sigma\{\text{Driver Torques}\} - \Sigma\{\text{Load Torques}\}$$

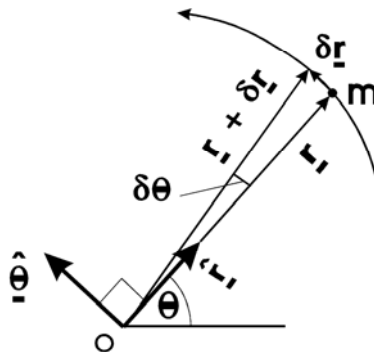


Figure 5.1: Mass Moving About A Central Point

For an object '**m**' moving about a fixed point '**o**', as shown above, the velocity can be expressed in terms of its position vector, i.e.

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{d}{dt}(r\hat{r}) \tag{58}$$

which, on expansion gives,

$$\mathbf{v} = \dot{r}\hat{\mathbf{r}} + r\dot{\theta}\hat{\boldsymbol{\theta}} \quad (59)$$

Where,

- \mathbf{r} = position vector of mass m (m)
- θ = angular displacement of position vector (radians)
- m = mass of object (kg)
- \mathbf{v} = mass velocity vector (m/s)
- $\hat{\mathbf{r}}$ = unit position vector, etc., refer to Figure 5.1 (units)

When m moves in a circular plane, the magnitude of its position vector is constant and, hence, \mathbf{v} is perpendicular to \mathbf{r} . Thus, by forming a dot product of equation (59) with $\hat{\mathbf{r}}$, it is seen that,

$$\dot{r} = 0 \quad (60)$$

and, consequently, equation (59) reduces to,

$$\mathbf{v} = r\dot{\theta}\hat{\boldsymbol{\theta}} \quad (61)$$

The *angular momentum* of an object is defined as the *cross product* of *position vector* and *linear momentum*, i.e.

$$\mathbf{L} = \mathbf{r} \times \mathbf{P} = \mathbf{r} \times m\mathbf{v} = m(r\hat{\mathbf{r}}) \times (r\dot{\theta}\hat{\boldsymbol{\theta}}) \quad (62)$$

$$\therefore \mathbf{L} = mr^2\dot{\theta}(\hat{\mathbf{r}} \times \hat{\boldsymbol{\theta}}) \quad (63)$$

$$\therefore \mathbf{L} = mr^2\dot{\theta}\hat{\mathbf{n}} = mr^2\omega\hat{\mathbf{n}} \quad (64)$$

Where,

\mathbf{L} = angular momentum (kg m²/s)

\mathbf{P} = linear momentum (kg m/s)

$\hat{\mathbf{n}}$ = unit vector normal to \mathbf{r} and $\boldsymbol{\theta}$

ω = angular speed (radians/s)

The *moment of inertia* for an object moving in a circular path about a central point is defined as,

$$I = mr^2 \quad (65)$$

$$\therefore \mathbf{L} = I\omega\hat{\mathbf{n}} \quad (66)$$

Rewriting in terms of *rotational speed* yields,

$$\mathbf{L} = 2\pi IN\hat{\mathbf{n}} \quad (67)$$

Where,

I = moment of inertia (kg m²)

N = revolutions per second (1/s)

We see from the main definition above that the rate-of-change of angular momentum is equal to the sum of the applied torques. Thus, on differentiating equation (67) and rearranging we obtain,

$$\frac{dN}{dt} = \frac{I}{2\pi I} (T_D - T_L) \quad (68)$$

Where,

T_D = torque applied to shaft by driver(kg m)
 T_L = torque exerted by load(kg m)

Power can be expressed in terms of *torque* and *speed*, i.e.

$$P = 2\pi NT \quad (69)$$

Thus, equation (68) can be rewritten in terms of power rather than torque to give,

$$\frac{dN}{dt} = \frac{I}{4\pi^2 IN} (P_D - P_L) \quad (70)$$

Where,

P_D = power delivered to the shaft by driver (W, J/s)
 P_L = power absorbed by load (W, J/s)

Equation (70) is in a convenient form for simulation purposes, and would normally be integrated by numerical methods.

A mechanical machine, such as a *compressor* or a *turbine*, could not of course be represented by a simple mass rotating about a fixed point. However, equation (70) is still valid providing the inertia I is correct for the particular machinery configuration, refer to Appendix E. It should be noted that, for a *coupled rotor* machine consisting of a number of drivers and loads, the inertias can be summed arithmetically providing they are mounted on the same shaft. If they are on different shafts, separated by a gearbox, then the inertias must all be referred to the same speed before they are summed, e.g. for a system where the reference speed is taken to be that of the drive shaft, the equivalent inertia referred to the drive shaft speed would be,

$$I_{D \text{ equivalent}} = I_D + \left(\frac{N_L}{N_D} \right)^2 I_L \quad (71)$$

The ratio of speed N_L to N_D would normally be fixed and equal to the gearbox ratio.

Equation (70) can readily be derived by considering the rate-of-change of *kinetic energy*.

For a *steam turbine* driver, the useful power developed is given by,

$$P_D = \eta_t W_s \Delta h \quad (72)$$

Where,

- W_s = mass flow of steam (kg/s)
 Δh = enthalpy drop from inlet to outlet (J/kg)
 η_t = efficiency of turbine (units)

For an *axial-flow compressor* say, acting on a gas which can be represented adequately as a polytropic process, i.e.

$$pV^n = \text{constant} \quad (73)$$

the power absorbed is given by,

$$P_L = \frac{Z_1 R T_1}{\eta_c (n-1)/n MW} \left[\left(\frac{p_{g2}}{p_{g1}} \right)^{(n-1)/n} - 1 \right] W_g \quad (74)$$

Where,

- MW = molecular weight (units)
 n = polytropic exponent (units)
 p_{g1} = inlet gas pressure (Pa)
 p_{g2} = outlet gas pressure (Pa)
 R = ideal gas constant (8314.3 J/kg-mole-°K)
 T_1 = inlet gas temperature (°K)
 V = volume of gas (m³)
 W_g = mass flow of gas being compressed (kg/s)
 Z_1 = inlet compressibility (units)
 η_c = efficiency of compressor (units)

APPENDIX

A**THE DIVERGENCE THEOREM**

The following is a statement of the *Divergence* or *Gauss Theorem*, proofs of which may be found in most advanced mathematical texts dealing with the vector calculus.

$$\iint_S \mathbf{A} \cdot d\mathbf{S} = \iiint_V \nabla \cdot \mathbf{A} \, dv \quad (\text{A1})$$

Where,

\mathbf{A} = vector function continuous on S ,

$\nabla \cdot \mathbf{A}$ = divergence of vector \mathbf{A} ,

and other symbols have meanings as defined in the main text.

APPENDIX B

THE SUBSTANTIVE DERIVATIVE**B.1 THE EULERIAN VIEWPOINT**

A fluid flow system may be considered as the motion of fluid particles. Such a system can be analyzed by assuming fixed spacial co-ordinates, say (x_a, y_a, z_a) within the velocity field but with time changing and, hence, expressing the velocity of particles passing this by point with respect to time. This approach is referred to as the *Eulerian* viewpoint. Thus, fluid velocity is represented as,

$$\mathbf{V}(x_a, y_a, z_a, t) \quad (\text{B1})$$

The Eulerian viewpoint is appropriate for analysing the velocity of a fluid particle observed by a stationary observer, e.g. as it flows past a stanchion of a river bridge.

B.2 THE LAGRANGIAN VIEWPOINT

An alternative to the Eulerian viewpoint is the *Lagrangian* viewpoint. In this system a particle is followed and its velocity is expressed with respect to its spacial co-ordinates which are themselves a function of time. Thus, fluid velocity is represented as,

$$\mathbf{V}(x(t), y(t), z(t), t) \quad (\text{B2})$$

The Lagrangian viewpoint is appropriate for analysing the velocity of a fluid particle observed by a moving observer, e.g. from a moving ship.

B.3 ACCELERATION OF A FLUID PARTICLE

The acceleration of fluid in a system can be deduced from Newton's second law of motion by considering the time rate of change of velocity of one particular particle. By using the fluid velocity field we will be required to adopt

the Lagrangian viewpoint. Thus, noting that the co-ordinates are functions of time, we may establish the acceleration by employing the chain rule for differentiation, as shown below,

$$\mathbf{a} = \frac{d}{dt} \mathbf{V}(x, y, z, t) = \left(\frac{\partial \mathbf{V}}{\partial x} \frac{dx}{dt} + \frac{\partial \mathbf{V}}{\partial y} \frac{dy}{dt} + \frac{\partial \mathbf{V}}{\partial z} \frac{dz}{dt} \right) + \left(\frac{\partial \mathbf{V}}{\partial t} \right) \quad (\text{B3})$$

Since the co-ordinates refer to any one particle, it is clear that the time derivatives of x , y and z must be equal to the respective scalar velocity components of any one particle. Hence,

$$\mathbf{a} = \left(\frac{\partial \mathbf{V}}{\partial x} V_x + \frac{\partial \mathbf{V}}{\partial y} V_y + \frac{\partial \mathbf{V}}{\partial z} V_z \right) + \left(\frac{\partial \mathbf{V}}{\partial t} \right) \quad (\text{B4})$$

The acceleration \mathbf{a} of a fluid particle is therefore expressed as a function of x , y , z and t , consequently, it is a field variable. Equation (B4) corresponds to a Lagrangian viewpoint.

The acceleration of fluid particles in a flow field can be considered to be the superposition of two effects represented by equation (B4) above. The first term in parenthesis represents change in a particle's velocity due to a change in its position, and is called the *convective* acceleration. Convective acceleration can occur in a steady-state situation, e.g. where a channel converges causing fluid acceleration due to area change. The second term represents acceleration due to unsteady change in the velocity field local to the particle and, hence, this is called *local* acceleration; it corresponds to an Eulerian viewpoint.

The differentiation performed in equation (B4) is called the *total* or *substantive* derivative and is sometimes represented as,

$$\mathbf{a} = \frac{D\mathbf{V}}{Dt} \quad (\text{B5})$$

and can be applied to a *scalar* or a *vector* field.

Where not explicitly defined, symbols have meanings as defined in the main text.

THE DYADIC PRODUCT

A *dyadic product* of two vectors \mathbf{a} and \mathbf{b} is a special form of *second order tensor*. The elements of the array form a set of products of the elements of the vectors. The dyadic product is represented as shown below,

$$\mathbf{ab} = \begin{bmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{bmatrix} \quad (\text{C1})$$

A dyadic is, in general, not commutative, i.e. $\mathbf{ab} \neq \mathbf{ba}$. It should be noted that a dyadic product is presented in written text as two vectors adjacent to each other without any multiplication operator in between.

APPENDIX **D**

THE NAVIER-STOKES EQUATIONS

The following is a simplified derivation of the Navier-Stokes Equations.

The *Differential Momentum Balance* equation,

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \rho \mathbf{V} \mathbf{V} - \rho \mathbf{g} + \Delta p + \nabla \cdot [\mathbf{T}] = 0 \quad (\text{D1})$$

can be simplified by use of the *Continuity Equation*. If diffusion effects can be considered negligible, equation (11) is simplified to,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{V}) \quad (\text{D2})$$

The first two terms of equation (D1) can be expanded as shown below,

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \rho \mathbf{V} \mathbf{V} = \rho \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \frac{\partial \rho}{\partial t} + \mathbf{V} \nabla \cdot (\rho \mathbf{V}) + (\rho \mathbf{V}) \nabla \cdot \mathbf{V} \quad (\text{D3})$$

Then, from equation (D2) it is seen that the second and third terms on the R.H.S. of equation (D3) sum to zero. Thus,

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot \rho \mathbf{V} \mathbf{V} = \rho \left\{ \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \nabla \cdot \mathbf{V} \right\} \quad (\text{D4})$$

Substituting the result of equation (D4) into equation (D1), we obtain,

$$\rho \left\{ \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \nabla \cdot \mathbf{V} \right\} = - \Delta p - \nabla \cdot [\mathbf{T}] + \rho \mathbf{g} \quad (\text{D5})$$

Equation (D5) is a *vector* equation which, together with the *scalar* equation (D2), provides four equations for the five unknowns: V_x , V_y , V_z , ρ and p . By including an *equation-of-state*,

$$p = f(\rho, MW, T) \quad (\text{D6})$$

which relates *Pressure to Density, Molecular Weight and Temperature*, we have a complete set of equations that together comprise the *Navier-Stokes Equations*; they represent the main governing equations of fluid dynamics. For systems where, for practical purposes, the fluid composition and temperature do not remain constant, additional equations are required to obtain a complete solution, refer to sections 2.0 and 3.0 above.

THE MOMENT OF INERTIA

The following is a definition of the *Moment of Inertia* for a solid body, derivations of which may be found in most texts dealing with Classical Mechanics.

$$I = \iiint_V r^2 \rho \, dv \quad (\text{E1})$$

Where r represents the distance from the axis of rotation to the elemental mass, ρdv .

APPENDIX

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