We are IntechOpen,
the world's leading publisher of Open Access books
Built by scientists, for scientists

6,900
Open access books available

186,000
International authors and editors

200M
Downloads

Our authors are among the

154
Countries delivered to

TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities

CLARIVATE ANALYTICS
BOOK CITATION INDEX
INDEXED

WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com

Dynamically Incompressible Flow

Christopher Depcik and Sudarshan Loya
University of Kansas, Department of Mechanical Engineering
USA

1. Introduction

Quite often, researchers model a flow as dynamically incompressible without realizing it. This version of the governing equations has been employed to model exhaust aftertreatment devices since the initial work of Vardi and Biller in 1968 (Vardi & Biller, 1968). The small channels in these devices, along with a relatively low flow rate of exhaust gases coming from the engine, promote laminar flow with a speed of approximately one to ten meters per second. This speed is well below the compressible threshold of around 100 m/s or a Mach number of 0.3. As a result, the chemical species equations can be decoupled from the energy equation promoting a computationally faster and easier to program numerical model. While this assumption is indeed valid in this example, only a few researchers have directly stated that the gas is being modeled as dynamically incompressible (Byrne & Norbury, 1993; Depcik et al., 2010). In fact, when this concept is mentioned, reviews of the main author's submitted work in this realm often come back confused as to its meaning. The reviewers wonder how a gas, which is inherently compressible, can be modeled as incompressible. The key wording for this type of situation is "dynamically" incompressible. To clarify this situation, this chapter provides a thorough investigation into this modeling phenomenon.

The efforts begin by explaining the threshold by which a gas can be treated as dynamically incompressible. Dynamic incompressibility differs from incompressibility $(\rho = \text{constant})$ by the fact that the density of the gas is considered as being *approximately* constant $(\rho \approx \text{constant})$. This small change in equal to approximately equal sign has a large bearing on the results. From this assumption, the governing equations of flow are re-derived adding in this assumption in order to provide the proper fundamental versions of these equations for modeling. Of significant importance, when the Law of Conservation of Energy is formulated, an Energy Equation paradox ensues. In particular, two apparently equally valid versions of this equation are found. From this result, this work provides a unique insight into this paradox and indicates the correct description. Moreover, the governing equation of chemical species is included in this chapter, as it not often presented in fluid mechanics books; however, it is important for modeling chemically reactive flow, such as the situation with catalytic exhaust aftertreatment devices.

After describing the governing equations, the failure of this approximation is presented in order for the reader to understand when a model can provide inaccurate results. Finally, this chapter documents a specific example that can lead to highly erroneous results if a modeler does not comprehend the influence of the dynamically incompressible assumption on

reacting flows. As a result, this chapter will provide a helpful tool for others when they begin their usage of this version of the fluid mechanics equations.

2. Law of conservation of mass

Conservation of mass is derived from a differential control volume as indicated in Fig. 1. The differential amount of mass (δm) given within the control volume is a function of the product of the fluid density (ρ) and volume (V):

$$\delta m = \rho \delta \mathbb{V} \tag{1}$$

with the differential volume indicated as:

$$\delta \mathbb{V} = dxdydz \tag{2}$$

It is important to note that all derivations that follow in this chapter, the differential control volume does not change with respect to time.

At each side of this control volume, a mass flux enters and exits the respective control surfaces as a function of local velocity conditions where u, v, and w represent the velocity in the x, y, and z directions respectively. The net mass flux is represented in the x-direction as shown in Fig. 1 as:

$$\text{Net Mass Flux}(x) = \left[\left(\rho u + \frac{\partial(\rho u)}{\partial x} dx \right) - \rho u \right] dydz = \frac{\partial(\rho u)}{\partial x} dxdydz \tag{3}$$
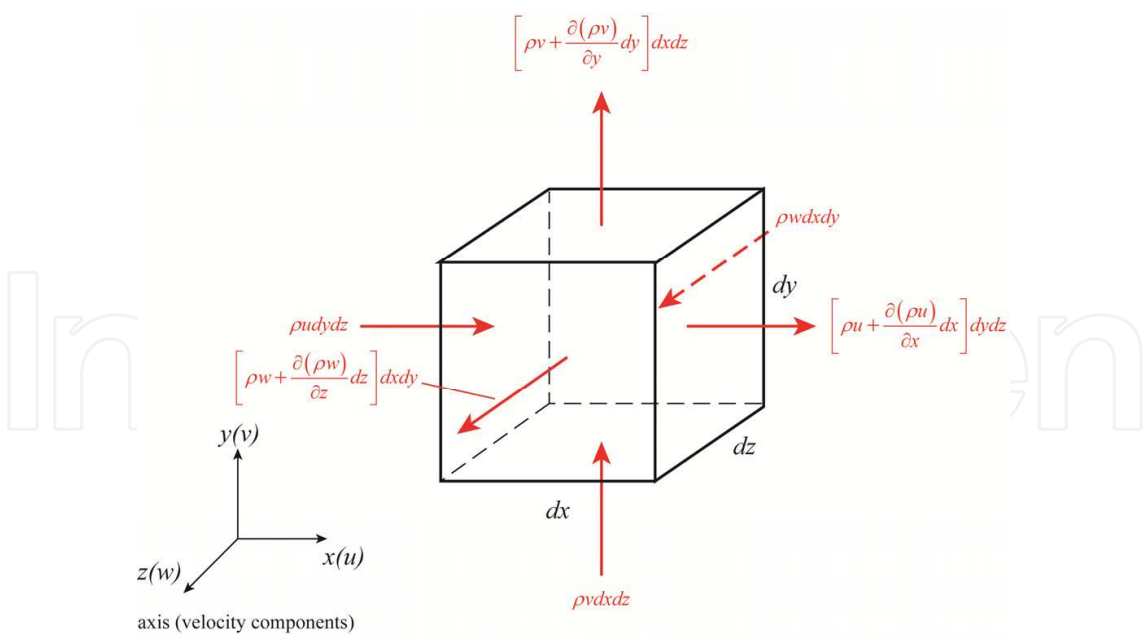

Fig. 1. Mass fluxes through a differential control volume.

In other words, the mass flux changes over the differential control surface in each direction are written as a function of its respective derivative in that direction. Hence, the change in mass flux in the x-direction in the previous equation is equal to:

$$\Delta(\rho u) = \frac{\partial(\rho u)}{\partial x} dx \tag{4}$$

with partial derivatives indicated because each variable is a function of all three dimensions. The change in slope of the x-direction mass flux is multiplied over the distance which the slope changes in order to calculate the difference in mass flux in that respective direction.

In the absence of nuclear reactions, conservation of mass states that there will not be a change in mass encompassing the control volume. Hence, the difference of mass within the control volume as a function of time is balanced by the net flow of mass through the control volume during a certain amount of time:

$$\frac{\delta m}{\delta t} + \sum \text{Net Mass Flux} = 0 \tag{5}$$

Written in differential format, this equation becomes:

$$\frac{\partial \rho}{\partial t} \delta \mathbb{V} + \left[\frac{\partial(\rho u)}{\partial x} dx\right] dy dz + \left[\frac{\partial(\rho v)}{\partial y} dy\right] dx dz + \left[\frac{\partial(\rho w)}{\partial z} dz\right] dx dy = 0 \tag{6}$$

Dividing through by the differential control volume, the conservation of mass is described as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \tag{7}$$

This can be written in vector format for simplicity as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \tag{8}$$

where the vector $\mathbf{V}$ is equal to $[u\ v\ w]$;

This version of the conservation of mass is known as the conservative formulation as all variables are embedded within the partial derivatives. However, it is often represented in non-conservative format by first expanding the derivatives:

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial v}{\partial y} + v \frac{\partial \rho}{\partial y} + \rho \frac{\partial w}{\partial z} + w \frac{\partial \rho}{\partial z} = 0 \tag{9}$$

and incorporating the definition of divergence in velocity along with the material derivative:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{V} = 0 \tag{10}$$

Both versions of the conservation of mass have their place in numerical analysis for incompressible and compressible flows. In this next section, the criterion for incompressible flow is described.

3. Mach number criterion

A fluid can either be considered incompressible or compressible depending on the interrelationship between pressure, density, velocity and temperature. Liquids and solids are nearly always incompressible as their density remains relatively constant independent of variations in these variables. An exact incompressible fluid has the properties of an infinite sound speed, where a pressure disturbance is felt everywhere within the fluid at each instant in time. Gases are compressible since their density changes as a function of pressure and temperature; often related through the ideal gas law. However, a fluid can be considered *dynamically incompressible* when the speed of sound (aka low-amplitude pressure waves) is significantly faster than the velocity of the working fluid. In this case, the pressure and temperature are not directly related to the density of the medium and a simplification of the governing equations can occur (Kee et al., 2003).

In the study of fluid dynamics, aerodynamicists define a non-dimensional parameter after Ernst Mach that relates the fluid velocity to the speed of sound:

$$M = \frac{\mathbf{V}}{a} \qquad (11)$$

This parameter helps normalize different working fluids and relate their effects to different flow conditions. As a result, here it will help designate the conditions of incompressible flow independent of the working fluid.

The conservation of mass, equation (8), assuming incompressible flow, results in the following governing equation:

$$\nabla \cdot (\rho \mathbf{V}) = 0 \qquad (12)$$

By explaining in one-dimension for simplicity, the advection component now equals:

$$\nabla \cdot (\rho \mathbf{V}) \to \frac{\partial (\rho u)}{\partial x} = 0 \qquad (13)$$

and further expanding the derivative in non-conservative format recovers:

$$\frac{\partial (\rho u)}{\partial x} = \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} = 0 \qquad (14)$$

For density to be constant, the second term must be small compared to the first term:

$$u \frac{\partial \rho}{\partial x} \ll \rho \frac{\partial u}{\partial x} \Rightarrow \frac{\delta \rho}{\rho} \ll \frac{\delta u}{u} \qquad (15)$$

A process of similarity can be used to compare both differential components in equation (15), given small changes in their respective components. This equation indicates that compressibility needs to be considered only when velocity variations are responsible for density variations.

The speed of sound (*a*) is given by the following thermodynamic relationship under isentropic situations:

$$a^2 = \left(\frac{\partial p}{\partial \rho}\right)_s \approx \frac{\delta p}{\delta \rho} \tag{16}$$

which is then converted similarly to equation (15) into small changes of the respective variables.

Pressure is then related to the velocity by using Bernoulli's equation for irrotational, one-dimensional flow when elevation changes are negligible:

$$\delta p \approx -\rho u \delta u \tag{17}$$

Combining the three equations elucidates the condition for velocity below which flow can be considered to be incompressible:

$$\frac{u^2}{a^2} = M^2 \ll 1 \tag{18}$$

Experimental observations indicate that the following condition can typically be assumed to indicate the limit of dynamically incompressible flow:

$$M \leq 0.3 \tag{19}$$

Therefore, when the Mach number is relatively small, it is reasonable to utilize the dynamic incompressibility assumption for the governing equations of fluid dynamics. From this result, the governing equation of continuity is simplified from equation (10) to:

$$\nabla \cdot \mathbf{V} = 0 \tag{20}$$

The divergence of velocity in this equation $(\nabla \cdot \mathbf{V})$ is the time rate change of volume of a moving fluid element, per unit volume. Equation (20) means that the change in volume (volume dilation) of the fluid element is zero. This result is consistent with equation (1); i.e., if density and mass are constant, the volume is required to be constant. Written out explicitly using directional variables, the divergence of velocity is given as:

$$\nabla \cdot \mathbf{V} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{21}$$

4. Law of conservation of momentum

Consider a fluid element subjected to body forces caused by gravitation, and to surface forces like pressure and shear stresses caused by fluid friction as shown in Fig. 2. From Newton's second law of motion, the time rate of change of momentum of a body ($m\mathbf{V}$) equals the net force ($\mathbf{F}$) exerted on it:

$$\mathbf{F} = \frac{d}{dt}(m\mathbf{V}) \tag{22}$$

where the left hand side represents the forces exerted on the body and the right hand side is the time rate of change and net flow of momentum within the control volume.
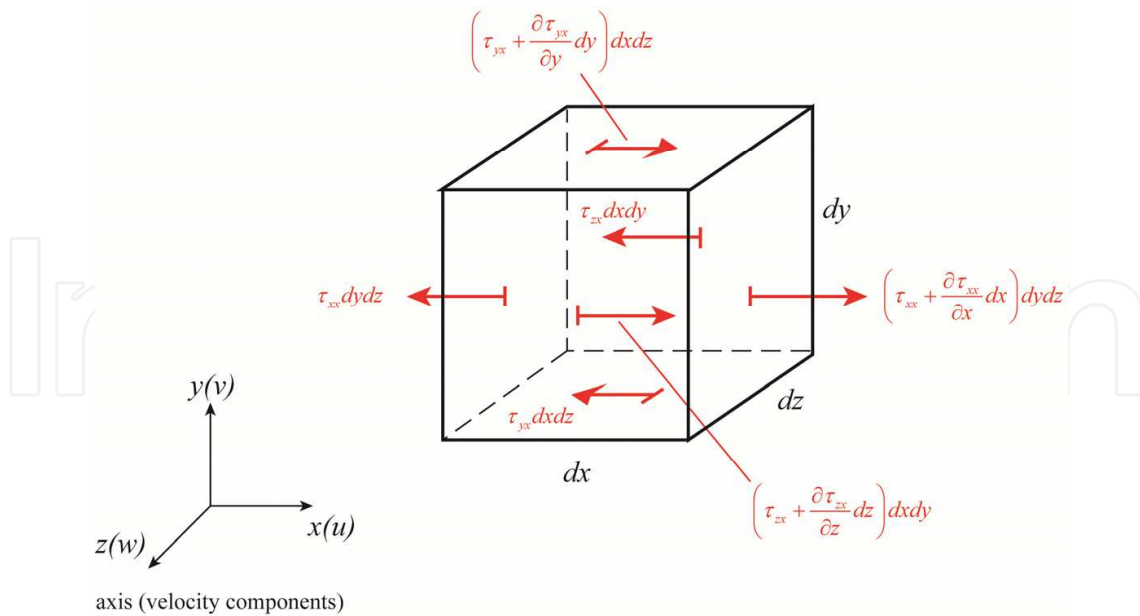
Fig. 2. Forces acting on a control volume, with only *x*-direction illustrated.

In the absence of external forces, the time rate of change of momentum inside the control volume would be balanced by the momentum flux entering the control volume during a certain amount of time (analogous to the conservation of mass):

$$\frac{\delta(m\mathbf{V})}{\delta t} + \sum \text{Net Momentum Flux} = 0 \tag{23}$$

Since the mass entering the control volume on each side brings along with it a respective amount of momentum from all three directions, the momentum flux can be derived in a similar manner as the net mass flux as:

$$\text{Net Momentum Flux}(x) = \left[\left(\rho u\mathbf{V} + \frac{\partial(\rho u\mathbf{V})}{\partial x}dx\right) - \rho u\mathbf{V}\right]dydz = \frac{\partial(\rho u\mathbf{V})}{\partial x}dxdydz \tag{24}$$

For example, the *x*-momentum equation would equal, in the absence of external forces:

$$\frac{\partial(\rho u)}{\partial t}\delta\mathbb{V} + \left[\frac{\partial(\rho uu)}{\partial x}dx\right]dydz + \left[\frac{\partial(\rho uv)}{\partial y}dy\right]dxdz + \left[\frac{\partial(\rho uw)}{\partial z}dz\right]dxdy = 0 \tag{25}$$

utilizing equations (1) and (23).
Hence, the total change of momentum inside the control volume for all three-dimensions via the right hand side of equation (22) equals:

$$\frac{d}{dt}(m\mathbf{V}) \rightarrow \frac{\partial(\rho\mathbf{V})}{\partial t}\delta\mathbb{V} + (\nabla \cdot \rho\mathbf{V}\mathbf{V})\delta\mathbf{S} \tag{26}$$

where $\delta\mathbf{S}$ is a vector indicating the control surface in the respective direction:

$$\delta S_x = dydz \; ; \; \delta S_y = dxdz \; ; \; \delta S_z = dxdy \tag{27}$$

The forces on this fluid element are broken up into those that act at a distance, caused by force fields acting through space proportional to the control volume (body), and shear and strain forces (surface) that include both normal and tangential components proportional to the area:

$$\mathbf{F} = \mathbf{F}_B + \mathbf{F}_S \tag{28}$$

where $\mathbf{F}_B$ are body forces and $\mathbf{F}_S$ are surface forces in the above equation.
Body forces in this case include only gravity:

$$\mathbf{F}_B = \left(\rho \delta \mathbb{V} \right) \mathbf{g} \tag{29}$$

where $\mathbf{g}$ is a vector oriented in the direction of the solved equation. Other body forces do exist like electromagnetic forces; however, these forces are beyond the scope of this chapter.
The surface forces act on the boundary of the control volume and are applied by external stresses on the sides of the element. Similar to the net momentum flux, a net stress component can be derived as indicated via Fig. 2 and equation (24)

$$\text{Net Stress}\left(x \right) = \frac{\partial \tau_{xx}}{\partial x} dx dy dz + \frac{\partial \tau_{yx}}{\partial y} dy dx dz + \frac{\partial \tau_{zx}}{\partial z} dz dx dy \tag{30}$$

where the first subscript on the stress component (τ) indicates the surface orientation by providing the direction of its outward normal and the second subscript indicates the direction of the force component.
In the absence of shear and strain, flow can and will happen because of the normal compressive stress exerted by the working fluid on the boundaries. This is called the hydrostatic pressure condition, as pressure force always acts normal and against the control surface in each direction. Hence, the stress tensor can be represented as:

$$\boldsymbol{\tau} = -p\delta_{ij} + \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} = -p\delta_{ij} + \boldsymbol{\tau}' \tag{31}$$

with the complete surface force represented as:

$$\delta \mathbf{F}_S = \boldsymbol{\tau} \cdot \delta \mathbf{S} \tag{32}$$

The rest of the stress tensor in equation (31) is calculated by considering the motion of a fluid element as it moves through a flow field. Fluids can undergo a number of different phenomena, as indicated in Fig. 3:

- Translation – linear movement from one location to another
- Rotation – the sides of the element may change as a function of pure rotation
- Angular deformation – distortion of the element by converting perpendicular planes to non-perpendicular planes
- Linear deformation – a change in shape without a change in orientation
- Volume dilatation – rate of change of volume per unit volume

Of these different influences, the last three relate to the strain that the fluid element undergoes. Only a brief summary of these components is presented in this section and the readers may wish to refer to the following references for a full derivation (Anderson, 1995; Schlichting & Gersten, 2000; Fox et al., 2004; White, 2003; Panton, 2005; White, 2006).
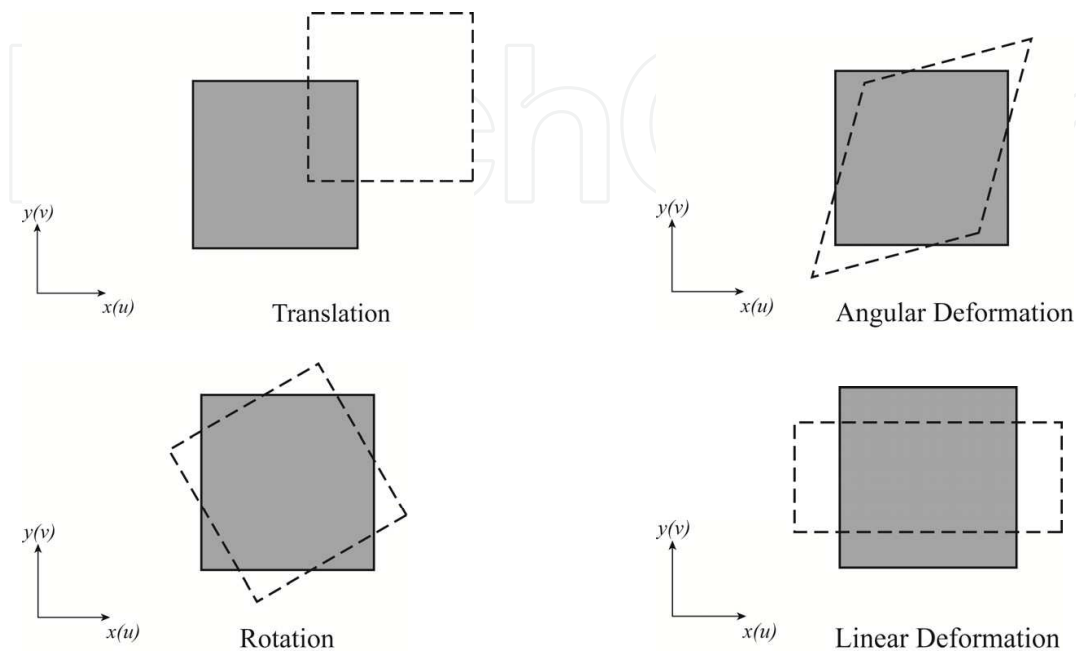

Fig. 3. Impact of fluid motion on fluid element as it flows through a flow field in two-dimensions.

Angular deformation occurs when the fluid element experiences a rate of deformation given by the change in velocity over the distance computed. In order to formulate a mathematical interpretation of this phenomenon, two assumptions are often made. The first relates to the assumption of a Newtonian Fluid, where the stress at a point is linearly dependent on the rates of strain (deformation) of the fluid. The second involves classifying the fluid as isotropic where the properties of the fluid are independent of direction of orientation. As a result, the components in the stress tensor that are a function of angular deformation are:

$$\tau_{yz} = \tau_{zy} = \mu\left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right); \ \tau_{xy} = \tau_{yx} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right); \ \tau_{zx} = \tau_{xz} = \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \tag{33}$$

where μ is a constant of proportionality that can be measured experimentally; also known as the dynamic viscosity.

Because of velocity gradients, the fluid element can deform as it moves. Linear deformation happens when the flow causes strain by stretching or shrinking the shape of the fluid element. Because of the isotropic condition previously specified, it was found that the linear coefficient of proportionality is equal to twice the constant of proportionality of angular deformation:

$$\tau_{xx,a} = 2\mu\frac{\partial u}{\partial x}; \ \tau_{yy,a} = 2\mu\frac{\partial v}{\partial y}; \ \tau_{zz,a} = 2\mu\frac{\partial w}{\partial z} \tag{34}$$

The fluid can also undergo a volumetric dilatation that equals the rate of change of the volume per unit volume. This component can be thought as the elasticity or compressibility of the working fluid, and while volume dilation and linear deformation are similar concepts, they are not the same. For example, a fluid element can undergo linear deformation (change in shape) but not necessarily volume dilation (change in volume). Similar to linear deformation, volume dilation does not involve any angular deflection and is purely linear in nature. Of interest, even though the fluid volume might only change in the x-direction, it does impact the other momentum equations. This is because the time-change component of the other momentum equations via equation (26) includes the density of the working fluid. Hence, even though the volume is changing only in the x-direction, it will influence the other governing equations through the density dependence. Moreover, because the isotropic condition is applied, the deformation is independent of the coordinate axis under which it is expressed. Therefore, the strain will impact all dimensions; hence, the normal component will be equal among all three dimensions:

$$\tau_{xx,b} = \tau_{yy,b} = \tau_{zz,b} = \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) = \lambda(\nabla \cdot \mathbf{V}) \tag{35}$$

The coefficient λ was originally considered independent of μ and is often called the second coefficient of viscosity in order to help differentiate volume dilation from angular deformation. In linear elasticity according to a Newtonian description, this variable is called Lamé's constant. For estimation of this variable, consult Gad-el-Hak for an understanding of the assumptions present in its calculation (Gad-el-Hak, 1995).

At this point, all phenomena have been developed and the momentum equations can be written out explicitly. The x-momentum equation expands to:

$$\frac{\partial(\rho u)}{\partial t}\delta\mathbb{V} + \left[\frac{\partial(\rho uu)}{\partial x}dx\right]dydz + \left[\frac{\partial(\rho uv)}{\partial y}dy\right]dxdz + \left[\frac{\partial(\rho uw)}{\partial z}dz\right]dxdy =$$
$$(\rho\delta\mathbb{V})g_x - \left(\frac{\partial p}{\partial x}dx\right)dydz + \left(\frac{\partial\tau_{xx}}{\partial x}dx\right)dydz + \left(\frac{\partial\tau_{yx}}{\partial y}dy\right)dxdz + \left(\frac{\partial\tau_{zx}}{\partial z}dz\right)dydz \tag{36}$$

and dividing through by the volume while making the assumption of incompressibility recovers:

$$\rho\left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} + u\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)}_{\nabla \cdot \mathbf{V} = 0}\right] = \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{yx}}{\partial y} + \frac{\partial\tau_{zx}}{\partial z} \tag{37}$$

Simplifying and incorporating the stress components equals:

$$\rho\frac{Du}{Dt} = \rho g_x + \frac{\partial}{\partial x}\left[-p + 2\mu\frac{\partial u}{\partial x}\right] + \frac{\partial}{\partial y}\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial z}\mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \tag{38}$$

Note that Lamé's constant does not appear in the above equation because the velocity gradient via equation (20) is approximately equal to zero. Therefore, the influence of Lame's

constant (λ) is ignored as it is multiplied by a negligible term; e.g. viscous stress is much smaller in magnitude than other flow parameters, like pressure, which results in the multiplication of a relatively small term by a negligible term.

For a Newtonian fluid, viscosity depends on temperature and pressure. In the case of a dynamically incompressible fluid, as discussed later, the change of temperature and pressure across the region must be relatively small in order for the assumption of dynamic incompressibility to hold. Hence, there is a negligible change in viscosity as a function of these parameters and the assumption of constant viscosity is valid.

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \mu \left[\underbrace{\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}}_{\nabla^2 u} \right] + \mu \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial y \partial x} + \frac{\partial^2 w}{\partial z \partial x} \right] + \rho g_x \tag{39}$$

By collecting the derivative in the second to last term on the right hand side, this results in:

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \mu \nabla^2 u + \mu \frac{\partial}{\partial x} \left[\underbrace{\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}}_{\nabla \cdot \mathbf{V} = 0} \right] + \rho g_x \tag{40}$$

Hence, this term disappears since the derivative of the velocity gradient is approximately equal to zero from dynamic incompressibility. Therefore, the final x-momentum governing equation for a dynamically incompressible flow equals:

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \mu \nabla^2 u + \rho g_x \tag{41}$$

Similarly, the momentum equations for dynamic incompressible flow in the y and z directions can be obtained as:

$$\rho \frac{Dv}{Dt} = -\frac{\partial p}{\partial y} + \mu \nabla^2 v + \rho g_y \tag{42}$$

$$\rho \frac{Dw}{Dt} = -\frac{\partial p}{\partial z} + \mu \nabla^2 w + \rho g_z \tag{43}$$

5. Law of conservation of energy

The physical principle governing the law of conservation of energy is that the total energy of the system must be conserved. Similar to the last two sections, consider a small fluid element moving with the fluid flow as in Fig. 4. The rate of change of total energy inside the fluid element (E) will be equal to the addition of the net heat flux (Q) into the element and rate of work done (W) on the fluid element due to body and shear forces. In mathematical form, this is represented as:

$$\frac{d}{dt}(mE) = \frac{dQ}{dt} - \frac{dW}{dt} \tag{44}$$

where heat transfer is defined as positive into the control volume and work is defined as positive out of the control volume.

The total energy inside the fluid element is a function of its internal energy, potential and kinetic energy due to the translational motion of the fluid element:

$$E = e + \frac{1}{2}\tilde{V}^2 + \mathbf{g} \tag{45}$$

where the effective kinetic energy velocity incorporates all three components of direction:

$$\tilde{V}^2 = u^2 + v^2 + w^2 \tag{46}$$

In the absence of heat transfer and work, the time rate of change of energy inside the control volume would be balanced by the energy flux entering the control volume during a certain amount of time (analogous to the conservation of mass):

$$\frac{\delta(mE)}{\delta t} + \sum \text{Net Energy Flux} = 0 \tag{47}$$

Since the mass entering the control volume on each side brings along with it a respective amount of energy from all three directions, the energy flux can be derived in a similar manner as the net mass flux as:

$$\text{Net Energy Flux}(x) = \left[\left(\rho uE + \frac{\partial(\rho uE)}{\partial x}dx\right) - \rho uE\right]dydz = \frac{\partial(\rho uE)}{\partial x}dxdydz \tag{48}$$
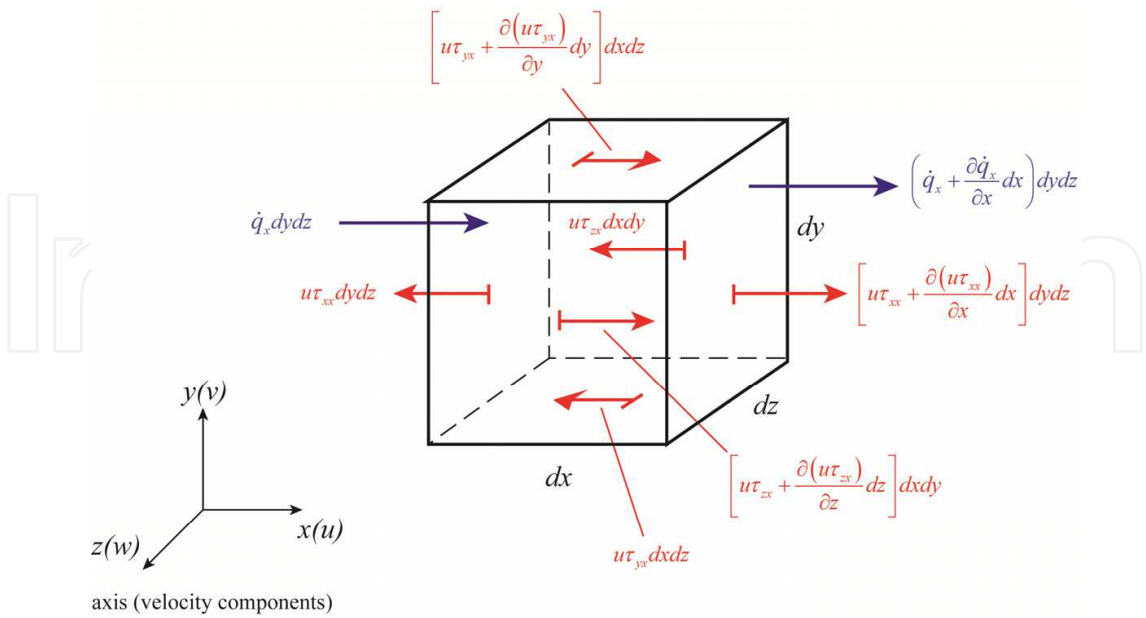

Fig. 4. Energy fluxes through an infinitesimally small fluid element with only the fluxes in the *x*-direction illustrated.

Hence, written in differential format, the left hand side of equation (44) becomes:

$$\frac{d}{dt}(mE) \rightarrow \frac{\partial(\rho E)}{\partial t}\delta\mathbb{V} + \left[\frac{\partial(\rho uE)}{\partial x}dx\right]dydz + \left[\frac{\partial(\rho vE)}{\partial y}dy\right]dxdz + \left[\frac{\partial(\rho wE)}{\partial z}dz\right]dxdy \qquad (49)$$

The net heat flux, as indicated in Fig. 4, incorporates a negative sign in order to account for the definition that heat transfer into the control volume is positive:

$$\text{Net Heat Flux}(x) = -\left[\left(\dot{q}_x + \frac{\partial\dot{q}_x}{\partial x}dx\right) - \dot{q}_x\right]dydz = -\frac{\partial\dot{q}_x}{\partial x}dxdydz \qquad (50)$$

Based on phenomenological evidence, Fourier found that the heat transfer rate in the direction per unit area perpendicular to the direction of transfer is linearly proportional to the temperature gradient in this direction. Furthermore, through the isotropic condition previously mentioned, all three directions incorporate the same proportionality constant, k, in determination of the heat flux:

$$\dot{q}_x = -k\frac{\partial T}{\partial x}; \quad \dot{q}_y = -k\frac{\partial T}{\partial y}; \quad \dot{q}_z = -k\frac{\partial T}{\partial z} \qquad (51)$$

This constant, referred hereto as thermal conductivity with a value that is a function of time, is analogous in its concept to viscosity in the momentum equation. Note that if the derivative of temperature is negative, heat transfer is positive as it is propagating in the forward direction (moving from hot to cold). Hence, the total net heat flux is equal to:

$$\frac{dQ}{dt} \rightarrow \left\{\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)\right\}dxdydz \qquad (52)$$

The work done on a fluid element is a function of the forces acting on this element. As indicated in the momentum equation, there are two forces (body and surface) evident. The rate of work done by a force is the product of this force and the component of velocity in the direction of the force. In order words, the time rate of work is equal to the force done over a certain distance as a function of time. Hence, the work done by the body force is represented as:

$$\text{Body Work} = (\rho\delta\mathbb{V})\mathbf{g}\cdot\mathbf{V} \qquad (53)$$

The rate of work done by the surface forces are the product of the stresses with the component of velocity in the corresponding direction. For example, the rate of work in the x-direction is equal to:

$$\text{Net Work}(x) = -\frac{\partial(u\tau_{xx})}{\partial x}dxdydz - \frac{\partial(u\tau_{yx})}{\partial y}dydxdz - \frac{\partial(u\tau_{zx})}{\partial z}dzdxdy \qquad (54)$$

including a negative sign as the force on the control volume is opposing the direction of the flow.

Including the work done by pressure and surface forces in all three directions, the total rate of work done is equal to:

$$\frac{dW}{dt} = -\left\{ \frac{\partial\left(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}\right)}{\partial x} + \frac{\partial\left(u\tau_{yx} + v\tau_{yy} + w\tau_{yz}\right)}{\partial y} + \frac{\partial\left(u\tau_{zx} + v\tau_{zy} + w\tau_{zz}\right)}{\partial z} \right\} dxdydz \quad (55)$$

And the governing equation for the conservation of energy, incorporating equations (49), (52) and (55) into equation (44) while dividing by the volume, equals:

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u E)}{\partial x} + \frac{\partial(\rho v E)}{\partial y} + \frac{\partial(\rho w E)}{\partial z} =$$

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + \quad (56)$$

$$\frac{\partial\left(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}\right)}{\partial x} + \frac{\partial\left(u\tau_{yx} + v\tau_{yy} + w\tau_{yz}\right)}{\partial y} + \frac{\partial\left(u\tau_{zx} + v\tau_{zy} + w\tau_{zz}\right)}{\partial z} + \rho(\mathbf{g}\cdot\mathbf{V})$$

which can be represented in vector format as:

$$\frac{\partial(\rho E)}{\partial t} + \nabla\cdot(\rho\mathbf{V}E) = \nabla\cdot(k\nabla T) - \nabla(p\mathbf{V}) + \nabla(\mathbf{V}\cdot\boldsymbol{\tau}') + \rho(\mathbf{g}\cdot\mathbf{V}) \quad (57)$$

with the pressure term separated out from the stress tensor as doing so will become important in a later section.

As a result, the energy equation governing fluid flow consists of two energy sources. Work through the body forces accelerates the fluid and increases its kinetic energy, while thermal energy conduction (heat flux) increases its internal energy (Panton, 2005). This equation can be further simplified by expanding the left hand side:

$$\rho\frac{\partial E}{\partial t} + \rho\mathbf{V}\cdot\nabla E + E\underbrace{\left[\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{V})\right]}_{0} = \nabla\cdot(k\nabla T) - \nabla(p\mathbf{V}) + \nabla(\mathbf{V}\cdot\boldsymbol{\tau}') + \rho(\mathbf{g}\cdot\mathbf{V}) \quad (58)$$

and incorporating the conservation of mass via equation (8) in order to recover:

$$\rho\frac{DE}{Dt} = \nabla\cdot(k\nabla T) - \nabla(p\mathbf{V}) + \nabla(\mathbf{V}\cdot\boldsymbol{\tau}') + \rho(\mathbf{g}\cdot\mathbf{V}) \quad (59)$$

Of importance, when the mechanical work component is subtracted from the total energy equation, the remaining part is called the thermal energy equation. As discussed earlier, mechanical work is equal to product of force and velocity. All the forces acting on the body are described via the momentum equation. Hence, in order to obtain the mechanical energy equation in the x-direction, one can multiply the momentum equation (37) (before simplifying this equation further) by the respective velocity component u as follows:

$$\rho\frac{D\left(u^2/2\right)}{Dt} = \left[-u\frac{\partial p}{\partial x} + u\frac{\partial\tau_{xx}}{\partial x} + u\frac{\partial\tau_{yx}}{\partial y} + u\frac{\partial\tau_{zx}}{\partial z} + \rho u g_x\right] \quad (60)$$

Similarly, the mechanical energy equations for the *y* and *z* directions can be found as:

$$\rho \frac{D(v^2/2)}{Dt} = \left[-v\frac{\partial p}{\partial y} + v\frac{\partial \tau_{xy}}{\partial x} + v\frac{\partial \tau_{yy}}{\partial y} + v\frac{\partial \tau_{zy}}{\partial z} + \rho v g_y \right] \tag{61}$$

$$\rho \frac{D(w^2/2)}{Dt} = \left[-w\frac{\partial p}{\partial z} + w\frac{\partial \tau_{xz}}{\partial x} + w\frac{\partial \tau_{yz}}{\partial y} + w\frac{\partial \tau_{zz}}{\partial z} + \rho w g_z \right] \tag{62}$$

By adding these equations, the total mechanical energy is obtained:

$$\rho \frac{D\left(\dfrac{\tilde{V}^2}{2}\right)}{Dt} = -\left(u\frac{\partial p}{\partial x} + v\frac{\partial p}{\partial y} + w\frac{\partial p}{\partial z} \right) + u\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right)$$
$$+ v\left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + w\left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) \tag{63}$$
$$+ \underbrace{\rho u g_x + \rho v g_y + \rho w g_z}_{\rho(\mathbf{g}\cdot\mathbf{V})}$$

which in vector format equals:

$$\rho \frac{D}{Dt}\left(\frac{\tilde{V}^2}{2} \right) = -\mathbf{V}\cdot\nabla p + \mathbf{V}\cdot\nabla\cdot\boldsymbol{\tau}' + \rho(\mathbf{g}\cdot\mathbf{V}) \tag{64}$$

When equation (45) is used in equation (59) and the derivitives are expanded on the right-hand side, the result is:

$$\rho \frac{D(e+\mathbf{g})}{Dt} + \rho \frac{D}{Dt}\left(\frac{\tilde{V}^2}{2} \right) = \nabla\cdot(k\nabla T) - p\nabla\cdot\mathbf{V} - \mathbf{V}\cdot\nabla p + \mathbf{V}\cdot\nabla\cdot\boldsymbol{\tau}' + \boldsymbol{\tau}':\nabla\mathbf{V} + \rho(\mathbf{g}\cdot\mathbf{V}) \tag{65}$$

The total mechanical energy from equation (64) can now be subtracted from the total energy equation, equation (65), in order to recover the thermal energy equation. Assuming that gravity has a negligible influence, the result is:

$$\rho \frac{De}{Dt} = \nabla\cdot(k\nabla T) - p\nabla\cdot\mathbf{V} + \boldsymbol{\tau}':\nabla\mathbf{V} \tag{66}$$

In order to utilize the thermal energy equation for modeling purposes, it is customary to convert it into temperature as the dependant variable (White, 2003). This conversion can be accomplished using either of two different methods as illustrated in the next section. As a result, an energy equation paradox results.

6. Energy equation paradox

Internal energy is a thermodynamic property that can be expressed by two fundamental properties of state. Here it is expressed in terms of temperature and specific volume:

$$de = \underbrace{\left(\frac{\partial e}{\partial T}\right)\bigg|_v}_{c_v} dT + \left(\frac{\partial e}{\partial v}\right)\bigg|_T dv \tag{67}$$

Note that the first term on the right hand side is the definition of the constant volume specific heat.

Substituting equation (67) in equation (66) finds:

$$\rho c_v \frac{DT}{Dt} + \rho \left(\frac{\partial e}{\partial v}\right)\bigg|_T \frac{Dv}{Dt} = \nabla \cdot (k\nabla T) - p\nabla \cdot \mathbf{V} + \boldsymbol{\tau}' : \nabla \mathbf{V} \tag{68}$$

However, the specific volume is reciprocal of density and, therefore equation (68) becomes:

$$\rho c_v \frac{DT}{Dt} + \left(\frac{\partial e}{\partial v}\right)\bigg|_T \left(-\frac{1}{\rho}\right)\frac{D\rho}{Dt} = \nabla \cdot (k\nabla T) - p\nabla \cdot \mathbf{V} + \boldsymbol{\tau}' : \nabla \mathbf{V} \tag{69}$$

Alternatively, internal energy can be expressed in terms of enthalpy as:

$$e = h - p/\rho \tag{70}$$

Written in derivative format, equation (70) becomes:

$$de = dh - dp/\rho + p\left(d\rho/\rho^2\right) \tag{71}$$

Since enthalpy is a thermodynamic property, it can additionally be expressed by two fundamental state variables; here, it is expressed as a function of temperature and pressure:

$$dh = \underbrace{\left(\frac{\partial h}{\partial T}\right)_p}_{c_p} dT + \left(\frac{\partial h}{\partial p}\right)_T dp \tag{72}$$

where the first term on the right hand side is the definition of the constant pressure specific heat of a fluid.

Using the basic law of thermodynamics along with Maxwell's relation,

$$\left(\frac{\partial h}{\partial p}\right)_T = \left[v + T\left(\frac{\partial s}{\partial p}\right)_T\right] = \left[v + T\left(\frac{\partial v}{\partial T}\right)_p\right] = \frac{1}{\rho}\left[1 - \frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p\right] \tag{73}$$

And substituting equations (72) and (73) into equation (71), one can write the internal energy as a function of the constant pressure specific heat:

$$de = c_p dT + \frac{1}{\rho}\left[1 - \frac{T}{\rho}\underbrace{\left(\frac{\partial \rho}{\partial T}\right)_p}_{\beta}\right]dp - \frac{dp}{\rho} + \frac{p}{\rho^2}d\rho \tag{74}$$

Note that the derivative of density with respect to temperature is the definition of the thermal expansion coefficient (β). In particular, a substance will expand with an increase in energy (heating) and contract with a decrease (cooling) with this dimensional response expressed as the coefficient of thermal expansion.

Furthermore, incorporating (74) into equation (66):

$$\rho\left[c_p\frac{DT}{Dt} - \frac{T\beta}{\rho}\frac{Dp}{Dt} + \frac{p}{\rho^2}\frac{D\rho}{Dt}\right] = \nabla\cdot(k\nabla T) - p\nabla\cdot\mathbf{V} + \mathbf{\tau}':\nabla\mathbf{V} \tag{75}$$

The terms in equation (75) can be rearranged and regrouped to produce:

$$\rho c_p\frac{DT}{Dt} = T\beta\frac{Dp}{Dt} - p\left[\underbrace{\frac{1}{\rho}\frac{D\rho}{Dt} + (\nabla\cdot\mathbf{V})}_{0}\right] + \mathbf{\tau}':\nabla\mathbf{V} + \nabla\cdot(k\nabla T) \tag{76}$$

Note that the expression in square brackets on the right hand side is the continuity equation for dynamically incompressible flow in non-conservative format and must therefore be equal to zero. As a result, the final thermal equation following this procedure equals:

$$\rho c_p\frac{DT}{Dt} = T\beta\frac{Dp}{Dt} + \mathbf{\tau}':\nabla\mathbf{V} + \nabla\cdot(k\nabla T) \tag{77}$$

As a result, equation (69) and equation (77) both represent the thermal energy equation utilizing temperature as the dependant variable. If one applies the assumption of dynamic incompressibility to both equations, the results are:

$$\rho c_v\frac{DT}{Dt} = \nabla\cdot(k\nabla T) \tag{78}$$

$$\rho c_p\frac{DT}{Dt} = \nabla\cdot(k\nabla T) \tag{79}$$

as the terms that were eliminated are negligible for an incompressible fluid.

In case of truly incompressible liquids and solids, the difference between the specific heat at constant volume and constant pressure vanishes. Hence, equation (78) and (79) reduce to a single equation:

$$\rho c\frac{DT}{Dt} = \nabla\cdot(k\nabla T) \tag{80}$$

However, because the specific heats of gases have distinct values equations (78) and (79) lead to a unique problem called the Energy Equation Paradox (White, 2003; Panton, 2005).

Both equation (78) and equation (79) cannot be simultaneously valid for the dynamically incompressible flow of gases. In particular, equation (78) implies that advection of internal energy is balanced by heat conduction, while equation (79) implies that enthalpy advection is balanced by heat conduction. In order to explain this paradox and obtain a solution, one

must first understand the assumption of dynamic incompressibility, its conditions and application in the governing equations.

Any gaseous flow is assumed to be incompressible if the velocity is less than a Mach number of 0.3 and there is not a large local change in temperature and pressure. For such a flow condition, density is assumed to be constant $(\rho = \text{constant})$ and the divergence of velocity is set equal to zero $(\nabla \cdot \mathbf{V} = 0)$. However, in actuality, there is a negligible change in density $(\rho \approx \text{constant})$ and divergence of velocity is not quite zero $(\nabla \cdot \mathbf{V} \approx 0)$. As a result, when the temperature gradient is not large, the conduction and advection of gases are relatively small and nearly of same magnitude as the divergence of velocity. Hence, in the thermal energy equation, any term containing the divergence of velocity or substantial derivative of pressure, temperature or density cannot be set immediately to zero without a thorough review.

6.1 Viscous dissipation

Viscous dissipation is always positive and acts to create internal energy (Panton, 2005). This change in energy is irreversible and it is written as a dyadic product of two tensors, shear stress and gradient of velocity $(\tau' : \nabla \mathbf{V})$ resulting in scalar work (Kee et al., 2003). Viscous dissipation describes rate of work for shape change at constant volume. For dynamically incompressible flow, change in shape at constant volume is negligible as density is assumed to be constant; hence, viscous dissipation is relatively small (Kee et al., 2003). Moreover, viscous dissipation becomes important when the fluid is highly viscous or turbulent (Kreith et al., 2010). In this case, the fluid is a gas with low viscosity under low Mach number situations. Therefore, the change in internal energy due to viscous dissipation will not influence the internal energy significantly and, subsequently, the temperature. As a result, it can be neglected in both equations (69) and (77).

6.2 Substantial derivative of pressure

The substantial derivative of pressure factor $\left[T\beta(Dp/Dt) \right]$ includes the thermal expansion coefficient, β. For an ideal gas, this coefficient is the reciprocal of temperature; hence, it cancels out the temperature component leaving just the material pressure derivative (Kundu & Cohen, 2010). For incompressible flow, thermodynamics properties (like k, c_p, μ) are often considered constant. Although they fundamentally change with temperature, one of the overriding assumptions for dynamic incompressibility is that there is not a substantial temperature change. If this assumption does not hold, the flow must be treated as compressible (Panton, 2005; Depcik et al., 2010). This assumption allows decoupling of the continuity and momentum equations from the thermal energy equation. Hence, all three velocities and pressure can be solved without needing to compute the temperature simultaneously. Therefore, the velocity field and pressure are unaffected by thermal changes in incompressible flow, since they are derived from the mass and momentum equations. Thus, pressure is represented as a force and not as a property influencing temperature. If the pressure increases or decreases across the incompressible flow region, the level of all pressures increases or decreases respectively. As a result, the change in pressure across the flow is negligible and it can be eliminated from equation (60).

6.3 Substantial derivative of density

For dynamically incompressible flow, the change in density is negligible. Moreover, any change in internal energy corresponding to a change in volume is marginal because the change in volume itself is small, as indicated in equation (21). Since this component is a product of two trivial terms, it is neglected in equation (69).

6.4 Pressure times divergence of velocity

Although the divergence of velocity may be small, pressure across the flow is significant in magnitude (Kee et al., 2003). Hence, this term is not inconsequential as the product is on the same order of scale as that of conduction: $p(\nabla \cdot \mathbf{V})$. As a result, applying the previous discussions and the influence of this component, the final thermal energy equation is obtained as a function of constant volume or constant pressure specific heats:

$$\rho c_v \frac{DT}{Dt} = \nabla \cdot (k\nabla T) - p(\nabla \cdot \mathbf{V}) \tag{81}$$

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot (k\nabla T) \tag{82}$$

In order to validate the previous discussion, the above two equations must generate the same results. Hence, the following derivation proves the methodology and explains the paradox.

For dynamic incompressibility, the change in density of a particle is negligible and therefore density is assumed constant. In mathematical form, this is represented as:

$$\frac{D\rho}{Dt} = 0 = \frac{1}{\rho}\frac{D\rho}{Dt} = \frac{1}{\rho}\frac{\partial \rho}{\partial p}\bigg|_T \frac{Dp}{Dt} + \frac{1}{\rho}\frac{\partial \rho}{\partial T}\bigg|_p \frac{DT}{Dt} \tag{83}$$

Since density is governed by the thermodynamic equation of state, it can be represented as a function of temperature and pressure (Panton, 2005). In addition, equation (83) can be written as:

$$\frac{1}{\rho}\frac{D\rho}{Dt} = \alpha\frac{Dp}{Dt} - \beta\frac{DT}{Dt} = 0 \tag{84}$$

where the isothermal compressibility 'α' and thermal expansion coefficient, β, are the characteristic of fluid and hence cannot be set to zero (Turcotte & Schubert, 2002; Graetzel & Infelta, 2002). However, if the change in pressure and change in temperature are sufficiently small, then equation (84) is equal to zero.

Incorporating equation (84) into equation (21):

$$-(\nabla \cdot \mathbf{V}) = \alpha\left(\frac{Dp}{Dt}\right) - \beta\left(\frac{DT}{Dt}\right) \tag{85}$$

As a result, equation (81) is modified to:

$$\rho c_v \frac{DT}{Dt} = \nabla \cdot (k\nabla T) + p\left[\alpha\left(\frac{Dp}{Dt}\right) - \beta\left(\frac{DT}{Dt}\right)\right] \tag{86}$$

For an ideal gas, isothermal compressibility 'a' is the reciprocal of pressure and the thermal expansion coefficient, β, is the reciprocal of temperature (Roy, 2001; Honerkamp, 2002; Kundu & Cohen, 2010). Incorporating these simplifications into equation (86) results in:

$$\rho\left(c_v + \frac{\beta}{\rho\alpha}\right)\frac{DT}{Dt} = \nabla \cdot (k\nabla T) + \frac{Dp}{Dt} \tag{87}$$

As explained earlier, the change in pressure across the flow is negligible and the substantial derivative of pressure in this equation is set to zero. Moreover, the specific heats of gases are related by the gas constant as:

$$c_p = c_v + R \Rightarrow c_v + \frac{p}{\rho T} \tag{88}$$

Using the property of isothermal compressibility and thermal expansion coefficient for ideal gases, equation (88) converts to:

$$c_p = c_v + \frac{p}{\rho T} = c_v + \frac{\beta}{\rho\alpha} \tag{89}$$

When equation (89) is used in equation (87), the result is identical to equation (79):

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot (k\nabla T) \tag{79}$$

This alternative development of equation (79) resolves the energy equation paradox; for dynamically incompressible flow, the advection of enthalpy is balanced by conduction.

7. Law of conservation of species

The law of conservation of species follows the same principles as the law of conservation of mass. At each side of the control volume indicated in Fig. 5, a species flux enters and exits the respective control surfaces as a function of local velocity conditions where u_A, v_A, and w_A represent the total species A velocity in the x, y, and z directions, respectively.

The net species flux is represented in the x-direction as shown in Fig. 5 as:

$$\text{Net Species Flux}(x) = \left[\left(\rho_A u_A + \frac{\partial(\rho_A u_A)}{\partial x}dx\right) - \rho_A u_A\right]dydz = \frac{\partial(\rho_A u_A)}{\partial x}dxdydz \tag{90}$$

where ρ_A is the density of the individual species considered.

Because reactions of chemical species may occur, the difference of mass of the species within the control volume as a function of time is balanced by the net flow of species through the control volume during a certain amount of time while including a local production or destruction rate:

$$\frac{\delta m_A}{\delta t} + \sum \text{Net Species Flux} = \dot{\omega}_A \delta \mathbb{V} \tag{91}$$

where the differential mass is written as:

$$\delta m_A = \rho_A \delta \mathbb{V} \tag{92}$$

and the chemical reaction rate has the units of kg m^{-3} s^{-1}, consumes species A when negative, and acts over the entire control volume. In differential format, equation (91) becomes:

$$\frac{\partial \rho_A}{\partial t}\delta\mathbb{V} + \left[\frac{\partial(\rho_A u_A)}{\partial x}dx\right]dydz + \left[\frac{\partial(\rho_A v_A)}{\partial y}dy\right]dxdz + \left[\frac{\partial(\rho_A w_A)}{\partial z}dz\right]dxdy = \dot{\omega}_A dxdydz \tag{93}$$
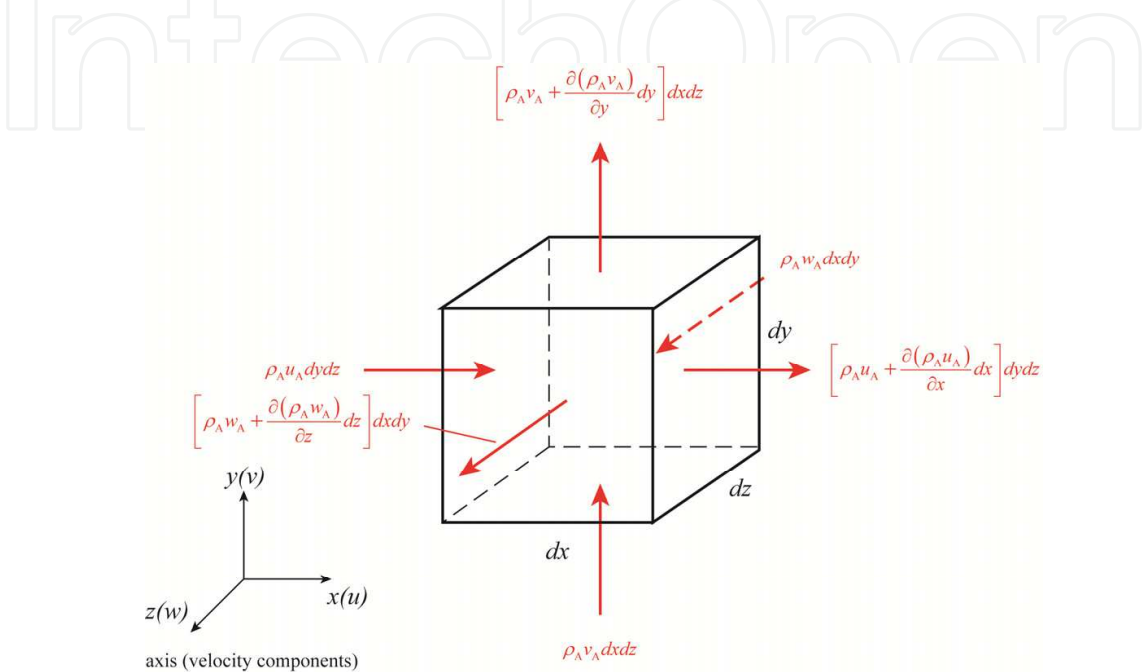
Fig. 5. Species fluxes through a differential control volume.

When equation (93) is divided through by $\delta\mathbb{V} = \delta x \delta y \delta z$, the differential control volume, the conservation of species A is described as:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial(\rho_A u_A)}{\partial x} + \frac{\partial(\rho_A v_A)}{\partial y} + \frac{\partial(\rho_A w_A)}{\partial z} = \dot{\omega}_A \tag{94}$$

This equation can be written in vector format for simplicity as:

$$\frac{\partial \rho_A}{\partial t} + \nabla \cdot (\rho_A \mathbf{V}_A) = \dot{\omega}_A \tag{95}$$

where the vector $\mathbf{V}_A$ is equal to $[u_A \ v_A \ w_A]$.

In this equation, the mass flux rate of individual species is the product of the specific density of that species and velocity in the given direction. However, the velocity of individual species depends not only on the bulk velocity of the flow, but also on concentration gradients. If there is a difference in concentration of species at various points across the flow, the species will move from regions of high concentrations to that of low concentrations. This motion is analogous to the phenomena of heat conduction from high temperatures to low temperatures. The velocity induced by a concentration gradient is called the diffusion velocity.

Consider a multicomponent system with different species in the mixture moving with different velocities in different directions. As shown in Fig. 6, **V** represents the mass averaged bulk velocity of the flow ($V = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$) and **V*** represents the molar averaged flow velocity. Both **V** and **V*** will differ in magnitude and direction as they contain unique weighing factors. Letting $\mathbf{V}_A$ be the velocity of species A, this value is independent on the molar weight or mass of the species A as it represents only that species. The difference between velocity of individual species and the mass averaged velocity is called the mass diffusion velocity of that species. In this case, it is $\mathbf{v}_A$. Similarly, the difference between individual species velocity and the molar averaged velocity of the flow is called the molar diffusion velocity $\mathbf{v}_A^*$.
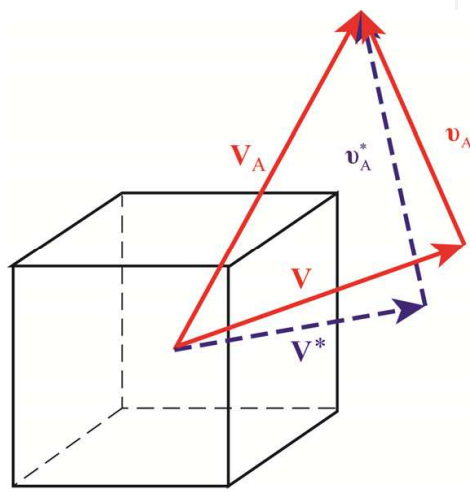
Fig. 6. Diagram of mass and molar averaged bulk velocity vectors.

Therefore, the velocity of individual species A is given as:

$$\mathbf{V}_A = \mathbf{V} + \mathbf{v}_A \tag{96}$$

Hence, the conservation of species equals:

$$\frac{\partial \rho_A}{\partial t} + \nabla \cdot (\rho_A \mathbf{V}) + \nabla \cdot (\rho_A \mathbf{v}_A) = \dot{\omega}_A \tag{97}$$

Adolf Fick investigated the diffusion velocity in the above equation in detail. He explained that $\mathbf{v}_A$ could be expressed using diffusion coefficients (δ). The use of this coefficient in the mass flux expression was later called Fick's law of diffusion and is written in mathematical format as:

$$\rho_A \mathbf{v}_A = -\rho_A \delta_{Am} \nabla (\ln Y_A) \tag{98}$$

where the mass fraction is given by

$$Y_A = \frac{\rho_A}{\rho} \tag{99}$$

with the *m* subscript on the diffusion coefficient indicating the value of species A with respect to the entire mixture as described later.

Substituting this expression back into Fick's law of diffusion:

$$\rho_A \mathbf{v}_A = -\rho_A \delta_{Am} \nabla \left(\ln \frac{\rho_A}{\rho} \right)$$

(100)

solving for the logarithmic derivative,

$$(\text{e.g., } \frac{\partial [\ln(\rho_A / \rho)]}{\partial x} = \frac{\rho_A}{\rho} \frac{\partial (\rho / \rho_A)}{\partial x}),$$

$$\rho_A \mathbf{v}_A = -\rho \delta_{Am} \nabla \left(\frac{\rho_A}{\rho} \right)$$

(101)

and substituting equations (99) and (101) into the conservation of species, equation (97), recovers:

$$\frac{\partial (\rho Y_A)}{\partial t} + \nabla \cdot (\rho Y_A \mathbf{V}) - \nabla \cdot (\rho \delta_{Am} \nabla Y_A) = \dot{\omega}_A$$

(102)

The first two components on the left hand side of equation (102) can be expanded to obtain,

$$\rho \frac{\partial Y_A}{\partial t} + \rho \mathbf{V} \nabla \cdot Y_A + Y_A \underbrace{\left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) \right]}_{0} - \nabla \cdot (\rho \delta_{Am} \nabla Y_A) = \dot{\omega}_A$$

(103)

and conservation of mass requires the term in square brackets of equation (103) to be zero so that:

$$\rho \frac{\partial Y_A}{\partial t} + \rho \mathbf{V} \nabla \cdot Y_A - \nabla \cdot (\rho \delta_{Am} \nabla Y_A) = \dot{\omega}_A$$

(104)

This equation is further modified as per the assumptions of dynamic incompressibility. Since the mass fraction of the species is related to the molar concentration of the species by:

$$Y_A = \frac{\bar{C}_A W_A}{\rho}$$

(105)

where W_A is the molecular weight of species A, the conservation of species equation for dynamic incompressible flow is:

$$\frac{\partial \bar{C}_A}{\partial t} + \mathbf{V} \nabla \cdot \bar{C}_A - \nabla \cdot \left(\delta_{Am} \nabla \bar{C}_A \right) = \frac{\dot{\omega}_A}{W_A}$$

(106)

Fick's law expresses the diffusion velocities in terms of diffusion coefficients. However, calculation of these coefficients has always been subject to interpretation in the literature. The standard method of calculating these values is a three-step process. First, the diffusion coefficient for one species is calculated as in a binary mixture consisting of two gases with one gas is held as the base. The binary diffusion coefficient is then calculated for all other

gases in the mixture, keeping the base gas constant. Then, the diffusion coefficient of the base gas is calculated for the mixture from all of the calculated binary diffusion coefficients. This method is then repeated for all the gases in the mixture keeping one gas as the base each time.

Many ways have been proposed to calculate the binary diffusion coefficient in the mentioned procedure (Perry & Green, 1984; Cussler, 1997; Kee et al., 2003; Kuo, 2005). After studying the referenced literature, the authors feel that binary diffusion between two species (A and B here) is best calculated by the following (Cussler, 1997; Kee et al., 2003):

$$\delta_{AB} = \frac{0.00186T^{1.5}\left(\dfrac{1}{W_A}+\dfrac{1}{W_B}\right)^{0.5}}{p\sigma_{AB}^2\Omega} \tag{107}$$

Equation (107) assumes all gases to be non polar, and although values of σ (Collision diameter of the molecule) and Ω (dimensionless energy integral based on temperature and Boltzmann constant) are not available for all gases. However, this equation provides for a relatively high accuracy, within an eight percent error range with experimental data (Cussler, 1997). This accuracy is appreciable as it is the closest any equation predicting binary diffusion coefficient can get. Even the commercial software program, transport CHEMKIN, supports this same equation for calculating these values (Reaction Design, 2003). From these binary coefficients, the mixture averaged diffusion coefficients can be calculated. The most accurate method to calculate these coefficients is to use a full multi-component system that involves inverting an L by L matrix, where L is number of species (Wilke, 1950; Perry & Green, 1984; Cussler, 1997; Kee et al., 2003). However, this method is computationally expensive and not required in most numerical models. As a result, most researchers use approximate formulas as follows.

When the mass diffusion velocity is given as a function of mass fractions,

$$\mathbf{v}_A = \frac{-1}{Y_A}\delta_{Am}\nabla Y_A \tag{108}$$

The mixture-averaged diffusion coefficient is represented as:

$$\frac{1}{\delta_{Am}} = \sum_{j\neq A}^{L}\frac{X_A}{\delta_{Aj}} + \frac{X_A}{1-Y_j}\sum_{j\neq A}^{L}\frac{Y_j}{\delta_{Aj}} \tag{109}$$

However, when the mass diffusion velocity is written using mole fractions (or molar concentrations),

$$\mathbf{v}_A = \frac{-1}{X_A}\delta'_{Am}\nabla X_A \tag{110}$$

The mixture-averaged diffusion coefficient is now written as:

$$\delta'_{Am} = \frac{1-Y_A}{\displaystyle\sum_{j\neq A}^{L}\frac{X_j}{\delta_{Aj}}} \tag{111}$$

The reason for the two different methodologies in calculating the diffusion coefficient relates to the solution of the mole or mass fraction version of the governing equation of chemical species. In specific, since mole and mass fractions are related by the molecular weight of the species, diffusion coefficients must be calculated differently in order to take this weighting factor into account. For more information on this topic, please consult the efforts of Kee et al. (Kee et al., 2003).

8. Failure of dynamic incompressibility

As discussed in the Mach Number Criterion section, when the pressure and temperature are not directly related to the density of the medium, one may simplify the governing equations via dynamic incompressibility (Kee et al., 2003). For catalytic exhaust aftertreatment modeling, a previous effort by the first author shows that traditional catalyst model equations assume dynamic incompressibility in order to simplify the solution technique by decoupling the species and energy equations (Depcik & Assanis, 2005). This model, represented by Figure 7, simulates an open channel interacting with the surface of the catalyst (washcoat impregnated with catalytic materials) by virtue of literature derived source terms, similar to equation (91), that model the interactions within the boundary layer. Use of dynamic incompressibility for simulating the gas in the open channel increases the computational speed of the model in order to make it suitable for transient regulatory tests and kinetic constant optimization.
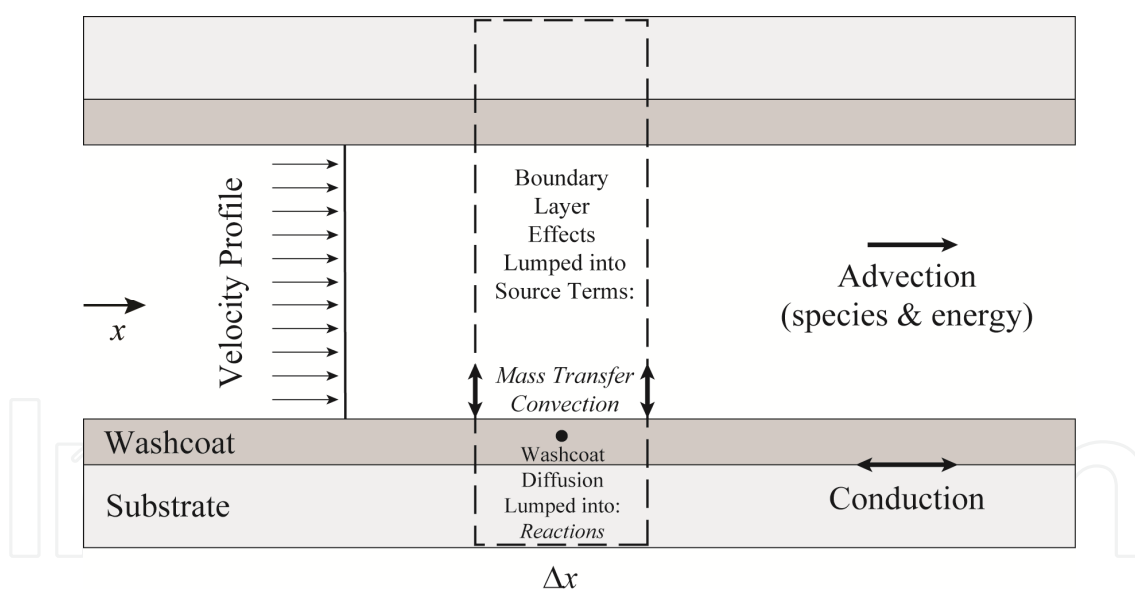

Fig. 7. One-dimensional catalytic exhaust aftertreatment model description.

Since the laminar channels of a monolithic catalyst do not contribute significantly to the pressure drop, the pressure throughout the catalyst is nearly constant. However, when a temperature profile exists, according to the ideal gas law the density must change along the monolith. This was stated previously by Byrne and Norbury (Byrne & Norbury, 1993) where they assert that the variation of gas density with temperature suggests that the flow should be treated as compressible for aftertreatment modeling; the assertion was further verified by Depcik et al. (Depcik et al., 2010). Compressibility leads to variations in velocity of the gas and a decreasing residence time of the gas in the catalyst.
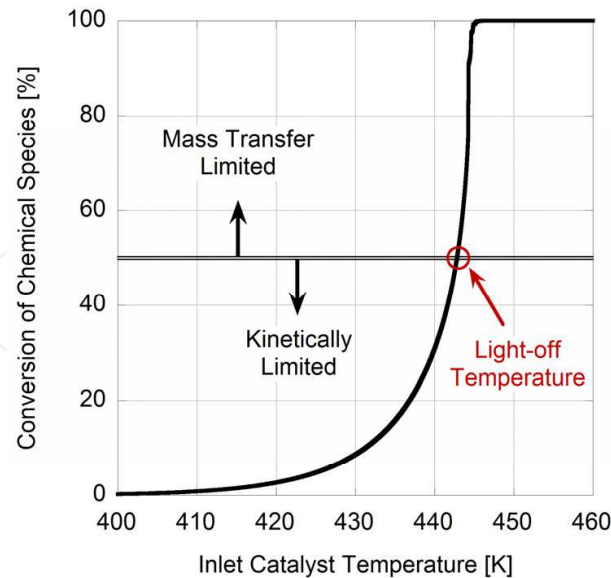
Fig. 8. Example of light-off temperature of a catalyst as indicated by the 50% conversion of the chemical species of interest.

One significant goal of the catalyst model is to simulate a "light-off event" when the catalyst transitions from kinetic to mass transfer regimes as illustrated in Figure 8. In other words, when the temperature is low, the reactions taking place on the surface are slow and there is little conversion of species across the catalyst (chemical kinetic limited). As the temperature increases, the reactions increase in magnitude until they hit a certain activation energy that causes an exponential jump in the magnitude of the conversion (50% conversion of inlet species is typically considered the light-off point). As a result, during a light-off experiment the temperature of the catalyst can change dramatically if a significant amount of exothermic reactions takes place. Hence, from a modeling standpoint, it becomes erroneous to employ dynamic incompressibility at this point. However, many researchers neglect this fact and continue to simulate the gas dynamics in this manner.

After light-off of a catalyst, it is commonplace to assume the reaction is now mass transfer limited and not kinetic limited. Hence, once entering the catalyst, all species will be converted. From a regulatory standpoint, modeling the catalyst after light-off is virtually unnecessary because most emissions occur in the cold start phase when temperatures and reaction speed is low (Koltsakis & Stamatelos, 1997). Therefore, during the times the model is most needed, pressure and temperature through the catalyst are relatively uniform; i.e. the use of dynamic incompressibility is valid.

As a result, it is important to understand that the assumption of dynamic incompressibility fails under situations that involve a significant pressure drop or temperature change. This failure occurs because the fluid is no longer held constant to the ideal gas law and the density remains independent of changes in pressure or temperature. However, by understanding the application of the model within certain parameters, it is possible to utilize dynamic incompressibility in a safe manner.

9. Reaction rate usage

One item that requires further discussion within the catalytic exhaust aftertreatment community is the use of mole fractions for reactions rates; e.g. the right hand side of equation (104). It must be stressed that reactions rates depend on concentration in principle. In the general case when the operation pressure can differ, the more suitable choice for formulating reactions rates is via concentration rate expressions because they inherently take into account changes in density. For example, consider a case of catalytic reactor working at one atmosphere. If reaction rates are expressed in terms of mole fractions, the reaction rate does not respond to the change of pressure. One obtains the same production rates even for a vanishing pressure. When the pressure is lowered, the subsequent production of species is slower because of a less dense mixture. Thus, a model not limited to a singular pressure must be based on concentration and take into account density variations; i.e. similar temperatures at different pressures would result in different densities but could have the same mole fractions. In other words, a model based on concentration can work for different operational pressures; whereas, a model based on mole fractions is fixed for one pressure.

Since pressure changes along the monolith are small and most automotive catalysts work at similar pressures, the use of mole fraction-based expressions does not cause significant problems, but it is important for the reader to understand the implication of doing so. If the reaction rate is written using concentration-based reaction expressions, the results will be significantly different because density is constant and does not respond to the temperature change, as discussed in the previous section; hence, reaction rates will be unique at each cell as axial temperature fluctuations change the calculated rate.

For a more in-depth discussion of this topic with respect to catalytic exhaust aftertreatment devices, please consult reference (Depcik et al., 2010). For simplicity, an example is given here for homogeneous (gas phase) reactions in order to demonstrate the concept. The right hand side of the compressible version of the chemical species equation (104), when homogeneous reactions occur, should be written in terms of the gas concentration

$$\dot{\omega}_A = A \exp\left(\frac{-E}{R_u T}\right) C_{CO} \tag{112}$$

where equation (112) expresses a linear reaction rate dependant on the species carbon monoxide according to the traditional Arrhenius rate expression.

However, when the dynamic incompressible version is used via equation (106)

$$\frac{\dot{\omega}_A}{W_A} = A \exp\left(\frac{-E}{R_u T}\right) X_{CO} \tag{113}$$

mole fractions must be used. The pre-exponential components (A) in both expressions can be equated at specific pressures and temperatures via density.

10. Conclusion

Dynamically incompressible flow is a convenient simplification of the governing equations of fluid mechanics in order to solve for flow conditions below a Mach number of 0.3. This assumption decouples the equations, because the fluid properties are no longer subject to

the constraint of the ideal gas law. Consequently, the equations can be solved in a reduced computational time. However, when pressure and temperature change significantly across the computational domain, the assumption of dynamically incompressible flow falters. In order to aid in the development of the reader, this chapter provided the proper background into this computational methodology and illustrated the correct tactic of computing reaction rates for the governing equation of chemical species.

11. References

Anderson, J. J. (1995). *Computational Fluid Dynamics: The Basics with Applications* (1st Ed), McGraw-Hill, 0070016852, New York.

Byrne, H. and J. Norbury (1993). Mathematical Modelling of Catalytic Converters. *Math. Engng. Ind.* vol. 4, no. 1, pp. 27-48.

Cussler, E. L. (1997). *Diffusion: Mass Transfer in Fluid Systems* (2nd Ed), Cambridge University Press, 0521450780, New York.

Depcik, C. and D. Assanis (2005). One-Dimensional Automotive Catalyst Modeling. *Progress in Energy and Combustion Science*, vol. 31, no. 4, pp. 308-369.

Depcik, C., A. Kobiera, et al. (2010). Influence of Density Variation on One-Dimensional Modeling of Exhaust Assisted Catalytic Fuel Reforming. *Heat Transfer Engineering*, vol. 31, no. 13, pp. 1098-1113.

Fox, R., A. McDonald, et al. (2004). *Introduction to Fluid Mechanics* (6th Ed), John Wiley & Sons, Inc., 0471202312, Hoboken, New Jersey.

Gad-el-Hak, M. (1995). Questions in Fluid Mechanics: Stokes' Hypothesis for a Newtonian, Isotropic Fluid. *Journal of Fluids Engineering*, vol. 117, no. 1, p. 3-5.

Graetzel, M. and P. Infelta (2002). *The Bases of Chemical Thermodynamics: Vol. 1*, Universal-Publishers, 1581127723.

Honerkamp, J. (2002). *Statistical Physics: An Advanced Approach with Applications* (2nd), Springer, 3540430202, Berlin.

Kee, R. J., M. E. Coltrin, et al. (2003). *Chemically Reacting Flow: Theory and Practice* (1st Ed), John Wiley & Sons, Inc., 0472361793, Hoboken, New Jersey.

Koltsakis, G. C. and A. M. Stamatelos (1997). Catalytic Automotive Exhaust Aftertreatment. *Progress in Energy and Combustion Science*, vol. 23, no. 1, p. 1-39.

Kreith, F., R. M. Manglik, et al. (2010). *Principles of Heat Transfer* (7th Ed), Cengage Learning, Inc., 0495667706.

Kundu, P. K. and I. Cohen (2010). *Fluid Mechanics* (4th Ed), Academic Press, 0123813999, New York.

Kuo, K. K. (2005). *Principles of Combustion* (2nd Ed), John Wiley & Sons, Inc., 0471046892, Hoboken, New Jersey.

Panton, R. L. (2005). *Incompressible Flow* (3rd Ed), John Wiley & Sons, Inc., 047126122X, Hoboken, New Jersey.

Perry, R. and D. Green (1984). *Perry's Chemical Engineering Handbook* (6th Ed), McGraw-Hill, Inc., 0070494797, New York.

Reaction Design (2003). *Transport Core Utility Manual*. Available from: http://eccentric.mae.cornell.edu/~laniu/MAE643/CHEMKIN3.7/transport.pdf

Roy, S. K. (2001). *Thermal Physics and Statistical Mechanics*, New Age International Publishers, 81-224-1302-1, New Delhi.

Schlichting, H. and K. Gersten (2000). *Boundary Layer Theory* (8th Ed), Springer, 3540662707, Berlin.

Turcotte, D. L. and G. Schubert (2002). *Geodynamics* (2nd), Cambridge University Press, 0521661862, New York.

Vardi, J. and W. F. Biller (1968). Thermal Behavior of an Exhaust Gas Catalytic Converter. *Industrial and Engineering Chemistry - Process Design and Development*, vol. 7, no. 1, p. 83-90.

White, F. (2003). *Fluid Mechanics* (5th Ed), McGraw-Hill, 0072402172, Boston.

White, F. (2006). *Viscous Fluid Flow* (3rd Ed), McGraw-Hill, 0072402318, New York.

Wilke, C. R. (1950). Diffusional Properties of Multicomponent Gases. *Chemical Engineering Science*, vol. 46, no. 2, p. 95-104.
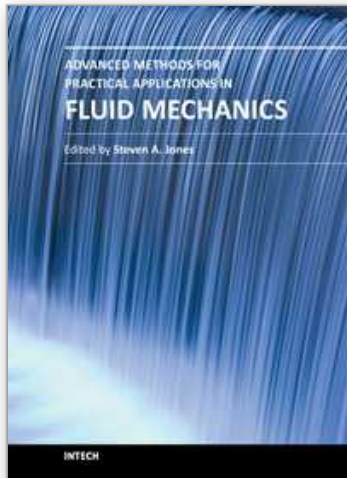
Advanced Methods for Practical Applications in Fluid Mechanics
Edited by Prof. Steven Jones

Whereas the field of Fluid Mechanics can be described as complicated, mathematically challenging, and esoteric, it is also imminently practical. It is central to a wide variety of issues that are important not only technologically, but also sociologically. This book highlights a cross-section of methods in Fluid Mechanics, each of which illustrates novel ideas of the researchers and relates to one or more issues of high interest during the early 21st century. The challenges include multiphase flows, compressibility, nonlinear dynamics, flow instability, changing solid-fluid boundaries, and fluids with solid-like properties. The applications relate problems such as weather and climate prediction, air quality, fuel efficiency, wind or wave energy harvesting, landslides, erosion, noise abatement, and health care.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

INTECH
open science | open minds