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Discrete flow and heat transfer patterns in low aspect ratio packed bed reactors

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Abstract

A 3-D network of voids (NoV) model was developed to study the discrete flow and heat transfer phenomena in multi-tubular packed-bed reactors. The model utilised does not place severe demands on computational resources. Hence, the model can probably easily be developed to simulate a fully packed tube and also a large number of tubes in the case of multi-tube reactors. Illustrative studies of the NoV model on a packed bed of spheres predict phenomenal variations of discrete angular velocities and consequently wall heat transfer coefficients within a single tube. The phenomenal variations of discrete wall heat transfer coefficients within a single tube imply that the different angular sections of the tube will transfer heat at radically different rates resulting in potentially large temperature differences in different segments of the tube. This may possibly result in temperature runaway and/ or hot spots development leading to several potentially unanticipated consequences for safety and integrity of the reactor.

Nomenclature

A_H	[m^2]	flow cross-sectional area
c_p	[Jkg^{-1}K^{-1}]	specific heat of fluid
d_i	[m]	void diameter
d_p	[m]	particle diameter
d_t	[m]	tube diameter
H	[m]	head loss
H_i	[m]	head loss in void i
ΔH	[m]	head correction
h_{wu}	[Wm^{-2}K^{-1}]	base case heat transfer coefficient
K_i		flow resistance constant in void i
k_f	[Wm^{-1}K^{-1}]	fluid conductivity
L_v	[m]	void length
N_p		number of axial planes
N_{Nu}		Nusselt number $\left(N_{Nu} = \dfrac{h_w d_i}{k_f} \right)$
N_{Re}		Reynolds number $\left(N_{\mathrm{Re}} = \dfrac{\rho_f u d_i}{\mu} \right)$
N_w		number of radial wedge segments
P_m	[m]	perimeter of a cross section
Q_i	[m^{3}s^{-1}]	flow rate in void i
Q_u	[m^{3}s^{-1}]	base case flow
r_c	[m]	radius of cylinder
r_H	[m]	hydraulic radius
u	[ms^{-1}]	void velocity
z	[m]	axial position in packed bed

Special Characters

μ	[kgm^{-1}s^{-1}]	fluid viscosity, kg/m-s
ρ_f	[kgm^{-3}]	density of fluid
θ	[radians]	angle of a radial wedge segment

Subscripts

c	cylinder
f	fluid
i	void number
j	plane number
w	wall voids

Introduction

Modelling of flow and heat transfer patterns in low aspect ratio packed bed reactors has so far been limited mostly to the use of global and mean quantities of voidage, velocity and heat transfer coefficients. Most of these models have been homogeneous or pseudo homogeneous in nature, whereas few models have considered the discrete fluid flow in the bed structure [1-3]. In low tube-to-particle diameter aspect ratio, wall effects are present across the entire bed and a more accurate description of flow behaviour can be obtained by discrete accounting for the invariably random variation of local bed geometry. This study shows that flow structure and heat transfer in low aspect ratio fixed bed reactors is better modelled by properly accounting for the discrete void fraction variations.

In order to understand the contribution of discrete random variation of voidage to issues such as parametric sensitivity and hot spots development different investigators have used different numerical methods such as computational fluid dynamics (CFD) and lattice-Boltzmann simulations. However, these approaches have been applied as yet to very small model systems due to the very severe computational resources demanded by such models [4-6]. Where attempt is made to model a fully packed tube, 2-D approaches have been utilised [7].

In this study, a representative typical sphere packing assembly is used to develop a three dimensional network of voids (NoV) model to investigate the contribution of discrete voidage variations to flow and heat transfer phenomena in packed-bed reactors. In principle, the network of voids model replicates both the geometry and structure of the voids space, so that flow through the network is equivalent to flow through the voids in the packed bed of spheres.

Void size determination

To characterise the flow behaviour in the void spaces it is necessary to define the void structure and size. The void structure is of arbitrary shape and has to be approximated by suitable void structure models. The packed bed of spheres in a cylindrical container is initially divided into a large number of wedge-shaped segments (N_w). The cylindrical wedge segments have identical width, $r_c\theta$, and equal height (L_v). If N_w is very high then a more detailed discrete distribution of angular porosity is obtained. On the other hand using small values of N_w has an averaging effect on the distribution of angular porosity. For clarity purposes the illustrated sphere packing assembly void structure and size used in this study is characterised by dividing by eight equally spaced planes in the axial direction as shown in **Figure 1**. Four planes are then used to discretise the packing radially and this results in eight segments. A typical plan view developed by radial discretisation at P1 will be as in **Figure 2.**

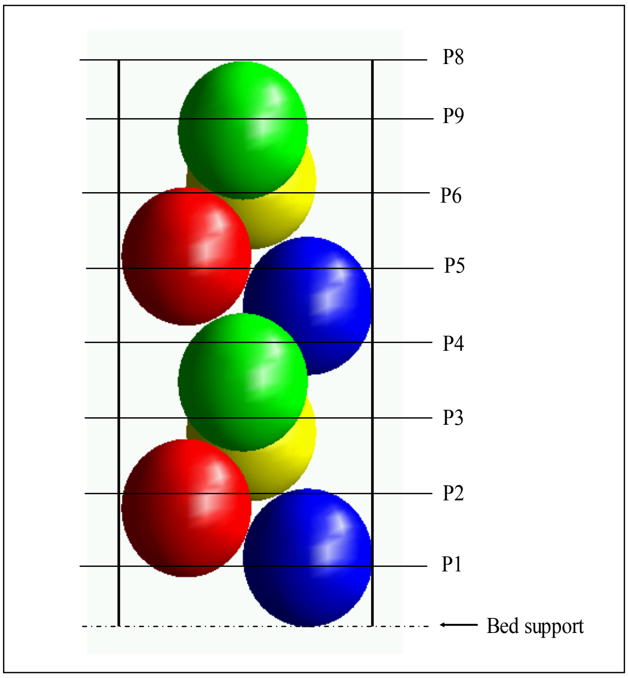

Figure 1 Eight equally spaced planes axially discretising the illustrated sphere packing assembly

The most common approach is to approximate the void structure as a set of cylindrical tubes. The voids equivalent radius can then be considered to be equal to the hydraulic radius of the void space available for flow [8, 9]. To account for any cross section presented to flow by a packed bed of spheres the hydraulic radius is defined as the ratio of the area of a cross-section to length of the perimeter of the cross-section, that is

$$r_H = \frac{A_H}{P_m} \tag{1}$$

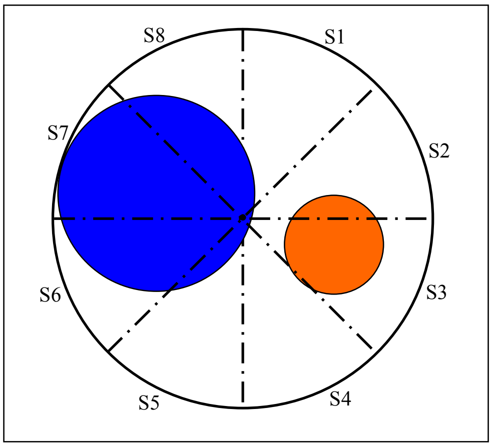

Figure 2 Eight radial segments at **P1** developed by radial discretisation of the packing with four vertical planes (eight radial segments)

Where, P_m is the perimeter of the cross section for flow and A_H is the cross sectional area available for flow in a radial wedge segment.

The length of a void, L_v, is taken to be the distance between two horizontally adjacent planes used to axially discretise the packing. It is found by subtracting the z coordinate of the *(j-1)* plane from the z coordinates of the j^{th} horizontal planes. The axial discretisation of the packing by eight planes implies that the distance from plane to plane will be 2.09×10^{-2}m and this is taken to be length of the voids (L_v) created. In essence, this length is an approximation of the true length travelled by a fluid element in the packed bed as the actual path of a given fluid element may be somewhat tortuous.

The resultant void size distribution after 8x8 discretisation of the illustrated sphere packing assembly is as shown in **Figure 3**. The dimensionless void sizes are obtained by dividing the diameter of the equivalent cylindrical conduits by the void length (L_v). The individual voids which form the network of voids show a wide variability. The maximum void size is about six times greater than the minimum void size. As void size influences the resistance a particular void offers to flow, the distribution of flow within the discrete voids will be expected to exhibit a similarly wide variation due to the wide variability in discrete void sizes.

Voids interconnection

The necessity of incorporating more detail in studying the influence of bed structure on fluid dynamics in fixed bed reactors without excessive computational requirements, precipitated the development of the network of voids analysis for a sphere packing assembly. The network of voids analysis offers simplicity in studying the influence of discrete angular voidage variations on fluid flow and heat transfer in fixed bed reactors. The discrete structure of the void space in which the fluid is transported can be completely defined once the sphere radius and positions are known. However, the void space is a continuous, interconnected region with a complex geometry. In the network-of-voids approach the packed bed is axially and radially discretised as described above and this results in a

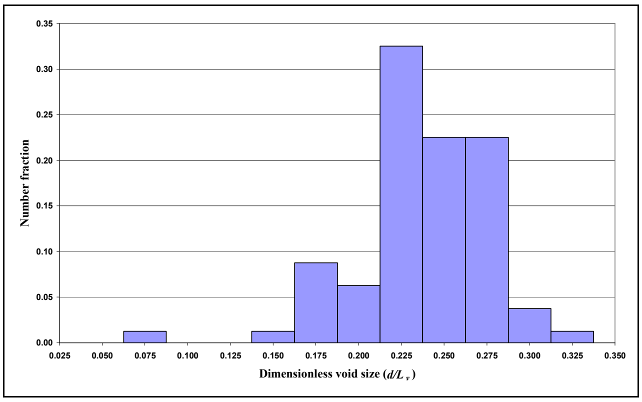

Figure 3 Dimensionless void size distribution for the illustrated sphere packing assembly for d_t/d_p = 1.93

packed bed with cylindrical wedge segments. The cylindrical wedge segments encompass the solids contribution of the spheres. Fluid flow within the packing will be in the void sections, that is the space not occupied by the solids. If the voids of the different axial and radial wedges are interconnected this results in a network-of-voids. The challenge is to obtain a network structure that can realistically approximate the fluid mechanics within the geometry of the sphere packing assembly.

The network-of-voids is developed by considering that axially and radially adjacent voids are in constant communication with each other. If flow through the packed bed is visualised to be from the bottom ($j = 1$) to the top ($j = N_p$) of the packing, then the voids in the first plane (bottom most) communicate with two radially adjacent voids and the void that is immediately above it in the axial direction. Voids between the bottom most and top most planes are interlinked to four adjacent void spaces and flow through the voids can be in any of these directions. The voids in the top most plane have a single upward out flow while voids radially adjacent to the node point void have flow in or out in either direction. At a given axial location, the fluid is taken to "virtually" transfer into or out of adjacent angular voids and this results in radial redistribution of flow creating the cross flows shown in **Figure 4** (a). By taking the transfer of fluid between adjacent angular voids as virtual, it implies that all cross flow voids offer little or no resistance to flow. Considering the fluid to flow from the bottom to the top of a packed bed the angular and axial voids can be taken to communicate as depicted in **Figure 4** (b).

Flow modelling using network analysis

Flow though the packed bed of sphere assembly could then be simulated using the established void size and the described void interconnections. The numerical computation of flow is governed by the fundamentals of network analysis of conserving mass and energy. Analysis of fluid flow in networks of conduits is mainly based on the analogy from Kirchoff's law applicable to electrical networks. If fluid flow in a network of conduits is made analogous to flow of electricity in networks then the following analogies become applicable:

I. The algebraic sum of the fluid flow into or out of any node should be zero.
II. The algebraic sum of the pressure head losses around any closed loop should be zero.

The first analogy is based on the continuity principle and the second analogy is the energy law. If volumetric flow rate is used with the continuity principle, the first analogy can be expressed mathematically as conservation, so that at a given junction

$$\left(\sum Q_i\right)_{out} = \left(\sum Q_i\right)_{in} \qquad (2)$$

Where, Q_i is the volumetric flow rate, and i denotes the conduit number. If a network of conduits contains J nodes and all external flows are known then (J-1) independent equations can be written using equation (2). The energy principle is satisfied by noting that if one adds the head losses around a closed loop, taking into account whether the head loss is positive or negative, the net head losses equal to zero. Mathematically, the energy principle gives L equations of the form

$$\sum^{L} H_i = 0 \qquad (3)$$

Neglecting losses other than friction, the characteristic equation for flow in conduits will be

$$H_i = K_i Q_i^{\,n} \qquad (4)$$

Where, K_i denotes a resistance constant of the specific i^{th} conduit and n is a constant whose value is dependent on the method used to evaluate the flow friction factor. Substitution of equation (4) into equation (3) gives

$$\sum_{n}^{L} K_i Q_i^{\,n} = 0 \qquad (5)$$

A network of conduits consisting of J nodes and L non-overlapping loops and M conduits will then satisfy the equation

$$M = (J-1) + L \qquad (6)$$

The (J-1) equations are linear although the associated L energy equations are non linear.

There are several commonly used numerical problem-solving methods applied to iteratively solve the flow or pressure distribution in networks of conduits. The nature of the flow problem in multi-tubular fixed beds configurations is such that the external flows into any given tube are not known before hand, necessitating the use of the Hardy Cross method also known as the single path adjustment method. There are two alternative procedures to the Hardy Cross relaxation method, which are the loop method, based on identity of head at a point, and the node method, based on continuity at a junction [10].

Multi-tubular fixed beds configuration favours the node approach as a fixed pressure drop can be set for each tube and the resultant discrete flow distribution analysed. The node method is an iterative procedure where initial head values at different nodes in the network are assumed. In this approach, the principal relationship used is the continuity equation. For each node in turn, the net total flow into the node is then calculated. If this is not zero, its head is corrected by an amount ΔH.

$$\Delta H = \frac{\sum Q_i}{\sum (Q_i / nH_i)} \quad (7)$$

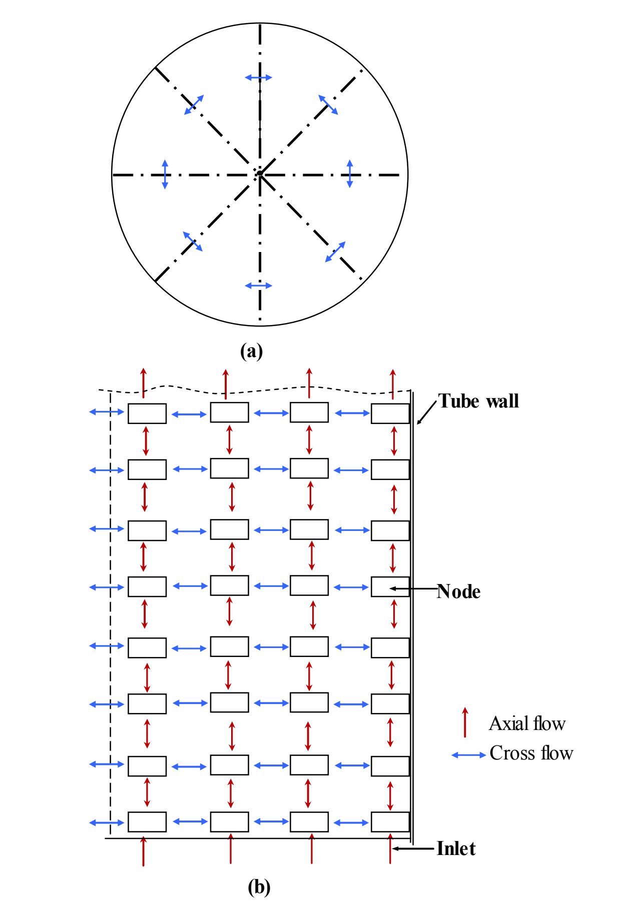

Figure 4 (a) Angular (tangential) voids communication **(b)** axial direction interaction of voids

Discrete modelling of wall heat transfer

For reactions with strong heat effects, low aspect ratio fixed bed reactors are normally employed to facilitate supply or removal of reaction heat. Due to the presence of close confining wall across the entire bed, it will be expected that the wall heat transfer process will greatly influence the behaviour of such reactors. Hence the need of discrete approaches that may give a better comprehension of operational issues such as hot spot development and parametric sensitivity associated with low aspect ratio fixed bed reactors.

In general, heat transfer inside packed beds can be through combinations of conduction, convection and radiation. These mechanisms combine and interact in a complex fashion within the complex geometry to produce the overall heat transfer behaviour in a packed bed reactor. The various near wall heat transfer mechanism can be classified into three groups[11]. The first group is made up of mechanisms that are based on the solid phase while the second and third group consists of mechanism through the voids that are either dependent or independent of fluid flow.

By transforming the illustrated sphere packing assembly to a NoV model, approximate discrete wall heat transfer coefficients could be evaluated using a simplified approach similar to that of analysing convective heat transfer inside conduits. This initial approach analysis focuses on heat transfer in discrete void spaces that is dependent on fluid flow and assumes that it is the major contributing heat transfer mechanism. When the flow Reynolds number in the discreet voids is laminar (N_{Re} < 2100), the discrete Nusselt numbers, N_{Nu}, are estimated using the classic correlation [12]. In the transition zone, N_{Nu} is evaluated using the recommended empirical correlation [13]. When the flow in the discrete voids becomes turbulent (N_{Re} > 10000), the discrete wall heat transfer coefficients could then be estimated using the appropriate modified equation [14].

Results and Discussions

The NoV model was used to investigate the contribution of variations of discrete voidage to flow and heat transfer patterns for a low aspect ratio packed bed with d_t/d_p=1.93 by applying a pressure drop of 1.0 Pa across the bed length. The simulations are based on the data for the catalytic oxidation of o-xylene [15]. **Table 1.0** shows the values of the different modelling parameters used for approximating the discrete flow and heat transfer coefficients in the reactor using the NoV model.

Table 1.0 Modelling parameters

Symbol	Value	Units
ρ_f	0.935	Fluid density, kg/m^3
μ	3.11x10^{-5}	Fluid viscosity, kg/m-s
c_p	1047	Specific heat of fluid, J/ Kg-K
k_f	4.35x10^{-2}	Fluid conductivity, W/m -K

Initially flow is simulated for the “base” case which assumes that all the discrete angular voids are equal to the packed bed overall mean voidage of 65.71%. In this case all the cross flows will have a zero magnitude due to the absence of a pressure gradient and the values of flow rates in the wall voids will be equal, this procedure is to some extent a validation procedure as well. The base case values of flow rates, velocity and heat transfer coefficients could then be used to make the different simulation results dimensionless.

To evaluate the influence of discrete voidage on the discrete flow a scatter plot of dimensionless flow rates and dimensionless void size is plotted in **Figure 5**. The discrete flow rates are made dimensionless by dividing the NoV model predictions flow rates by the base case flow rate (Q_u = 2.29x10^{-7}m^3/s). From the plot, discrete voids with high values exhibit both high and low flow rates. On the other hand, discrete voids with low size values also show both high and low flow rates as well. Hence, no clear relationship between the void size and the discrete void flow rate could be established. The absence of any meaningful trends between discrete void size and the discrete flow rates is indicative that at any node flow may be distributed in any of the interconnecting voids on the basis of the resistance the voids at that particular node offer to flow.

The overall fluid flow behaviour within the network is illustrated in the form of a discrete dimensionless voids velocity quiver plot in **Figure 6**. In the plot the arrow length and direction is indicative of increasing values of discrete dimensionless void velocity in particular regions bounded by the radial and axial planes. The discrete velocity structure has a complex pattern which shows cross voids velocities to have smaller magnitudes as compared to the discrete wall values. High axial velocities dominate with some isolated cases of high velocities in the cross flows voids being encountered within the network.

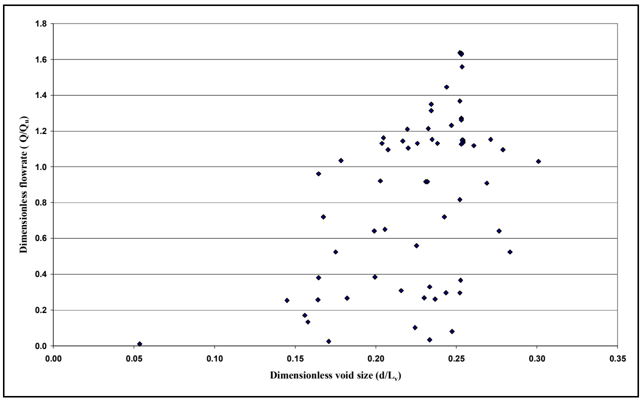

Figure 5 Scatter plot of discrete dimensionless flow rates against dimensionless void size of voids

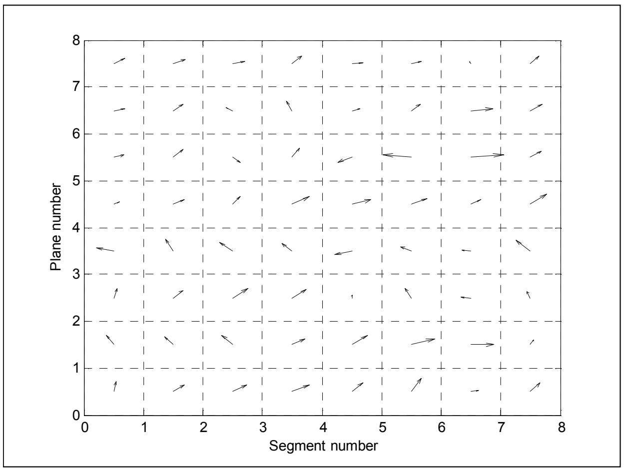

Figure 6 Dimensionless velocities in the different sections bounded by the radial and axial planes of voids

The distribution of dimensionless discrete wall heat transfer coefficients is plotted as a histogram in **Figure 7**. The dimensionless discrete wall heat transfer coefficients are obtained by dividing the NoV model predictions wall heat transfer coefficients by the wall heat transfer coefficient (h_{wu} = 11.70 W/m^2-K) predicted by the model for the base case. About 64.0% of the dimensionless discrete wall heat transfer coefficient values are close to h_{wu}. However, there are isolated incidences when the discrete wall heat transfer coefficients are either extremely low or high. For instance the maximum dimensionless discrete wall heat transfer coefficient is almost five times greater than the minimum dimensionless discrete wall heat transfer coefficient.

A qualitative comparison of the dimensionless discrete wall heat transfer coefficient values in the different regions bounded by radial and axial planes is visualised in **Figure 8.** The visual variation of dimensionless discrete wall heat transfer coefficients is from two opposite viewpoints which are 0^o and 180^o. The figure is a filled contour map wrap-around of the dimensionless discrete wall heat transfer coefficients on the wall of the containing vessel. Values represented by white are close or equal to h_{wu}, while values in the blue region are the discrete wall heat transfer coefficients that are below h_{wu} with deep blue indicating the lowest heat transfer coefficient. Values represented by shades of red are for discrete voids heat transfer coefficients higher than h_{wu}.

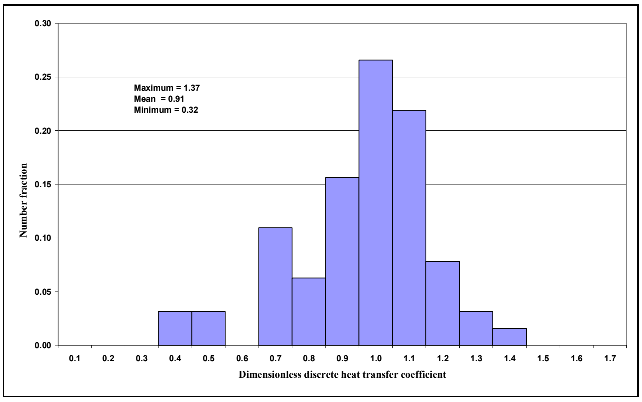

Figure 7 Distribution of dimensionless discrete wall heat transfer coefficients

The occurence of radically different values of discrete wall heat transfer coefficients within a single tube imply that the different sections of the tube will transfer heat at radically different rates, resulting in potentially large temperature differences in different segments of the tube. It will be expected that segments with low heat transfer will have a high chance of developing hot spots due to poor heat transfer rates in the case of highly exothermic reactions. Whereas the opposite cases when the wall heat transfer coefficients are relatively high imply better heat flux in that region and probably better conversion in such regions in the case of endothermic reactions.

Conclusions

A network of voids model that offers simplicity in incorporating the discrete variations of voidage for discrete fluid flow structure characterisation and does not require a massive computational effort has been developed. The NoV model predicts wide distributions of discrete flow rates within a single packed bed tube. The magnitude of the discrete flow rates in the voids has been established to be independent of the discrete void size. This is because the discrete flow behaviour of a given void is interdependent on the behaviour of voids interconnecting it and cannot be characterised in isolation. The distribution of discrete voids velocities shows a wide variability and

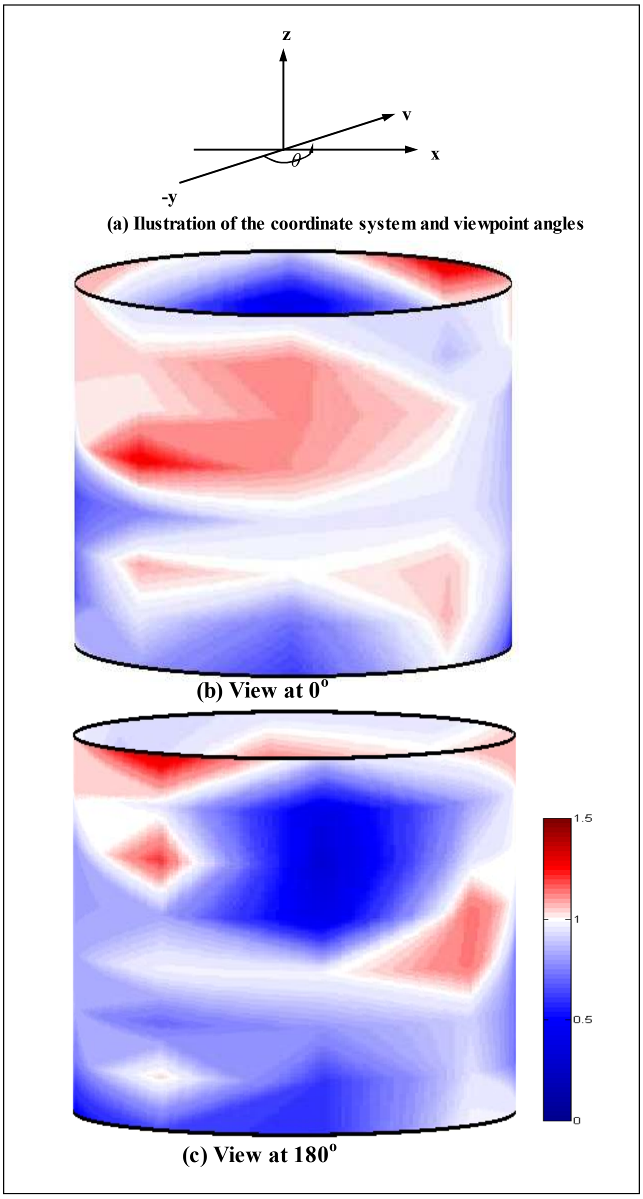

Figure 8 Variation of dimensionless discrete wall heat transfer coefficients

existence of low and high velocity gradients. Phenomenal variations of discrete wall heat transfer coefficients within a single tube are encountered and imply that the different discrete sections of the tube will transfer heat at radically different rates. This can potentially result in localised hot spots, with several potentially unanticipated consequences for safety and integrity of the reactor.

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