



This item was submitted to Loughborough's Institutional Repository (<https://dspace.lboro.ac.uk/>) by the author and is made available under the following Creative Commons Licence conditions.



**CC creative commons**  
COMMONS DEED

**Attribution-NonCommercial-NoDerivs 2.5**

**You are free:**

- to copy, distribute, display, and perform the work

**Under the following conditions:**

**BY:** **Attribution.** You must attribute the work in the manner specified by the author or licensor.

**Noncommercial.** You may not use this work for commercial purposes.

**No Derivative Works.** You may not alter, transform, or build upon this work.

- For any reuse or distribution, you must make clear to others the license terms of this work.
- Any of these conditions can be waived if you get permission from the copyright holder.

**Your fair use and other rights are in no way affected by the above.**

This is a human-readable summary of the [Legal Code \(the full license\)](#).

[Disclaimer](#) 

For the full text of this licence, please go to:  
<http://creativecommons.org/licenses/by-nc-nd/2.5/>

# COMPUTATIONAL MODELLING OF TWO-PHASE POROUS FLOW: “EFFECTS OF TEMPERATURE ON DYNAMIC CO-EFFICIENTS”

Navraj Hanspal & Diganta Bhushan Das  
School of Mechanical, Aerospace & Civil Engineering [MACE]  
Energy, Environment & Climate Change Group  
University of Manchester, M60 1QD, UK  
Email: navraj.hanspal@manchester.ac.uk

## KEYWORDS

Darcy's Law,  $P_c$ - $S$ - $K_r$  relationships, Dynamic Coefficient, Perchloroethylene (PCE)-Water system, STOMP

## ABSTRACT

Traditional continuum scale models for multiphase flow in porous media rely upon “Capillary Pressure, Saturation & Relative Permeability” relationships which do not necessarily illustrate the dynamic capillary pressure effects on the flow behaviour. As such, simulators for multiphase flow in porous media must include additional terms(s) associated with dynamic capillary pressures. For such reasons, investigations targeting at measurements of dynamic coefficients and its dependency on various physical parameters are of great interest. In this work we therefore examine the dependence of the dynamic coefficient  $\tau$  on temperature  $T$  by carrying out quasi-static and dynamic flow simulations for an immiscible perchloroethylene (PCE)-water system exhibiting a drainage process. Simulations are carried out using a two-phase porous media flow simulator STOMP for a range of temperatures between 20°C-80°C on 3-D cylindrical domains which correspond to laboratory scale domain set-ups used previously by the authors. Results are presented for coarse and fine sands at 40°C and are interpreted by examining the correlations between dynamic coefficient(s) and temperature, time period(s) required for attaining residual saturation and the dynamic aqueous/non-aqueous phase saturation and capillary pressure plots. Our simulations maintain a continuity from our previous work and reduce the inconsistencies associated with the dependency of dynamic coefficient(s) on temperature which should subsequently enable the users to carry out computationally economical and reliable modelling studies at various length scales of observation.

## INTRODUCTION

Immiscible displacement of non-aqueous phase liquids (NAPL) is of common occurrence in various subsurface flows, namely groundwater remediation methods and in oil recovery processes, which are of importance to the chemical, environmental, and petroleum sectors. Conventional approaches for continuum scale modeling of immiscible two-phase flow in porous media involve the use of extended version of Darcy's law (Darcy 1856, Muskat *et al* 1932; Scheidegger 1974, Whitaker 1986a and Hanung 1997) for multiphase flows in conjunction with the use of constitutive relationships between “Capillary Pressure, Saturation & Relative Permeability [ $P^c$ - $S$ - $K_r$ ]” based on quasi-static conditions (Bear and Verrujit, 1987; Helmig, 1997). These  $P^c$ - $S$ - $K_r$  relationships are highly non-linear in nature and depend on flow hydrodynamics (dynamic/static) conditions,

capillary or viscous forces, contact angles, grain size distribution, micro-scale heterogeneities, surface tension, boundary conditions, fluid properties, and length scales of observation. The conventional empirical macroscopic relations of the capillary pressure are functions of wetting phase saturation ( $P^c$ - $S$  relationships) and differences between the average pressures for oil/non-wetting and the water/wetting phase (Bear & Verrujit 1987; Helmig 1997) which can be mathematically expressed as,

$$P_{nw} - P_w = P^{c, equ}(S) = f(S) \quad (1)$$

where  $P_{nw}$  is the average pressure for oil/non-wetting phase and  $P_w$  is the average pressure for water or wetting phase,  $S$  refers to the water or wetting phase saturation. Equation (1) exhibits a linear-relationship between the saturation and capillary pressure which is obtained under steady-conditions in fluid equilibrium when saturation remains unchanged with time, considering all the aspects that affect the flow behaviour in porous media such as; material properties (e.g., porosity, intrinsic permeability, pore size distribution, etc), fluid properties (densities, viscosities, interfacial tensions, etc.), contact angles, wettability and the media heterogeneity. Steady state  $P^c$ - $S$ - $K_r$  relationships have been previously studied by various authors such as Beliaev & Hassanizadeh 2001; Beliaev & Schotting 2001; Murdoch & Hassanizadeh 2002; Hassanizadeh *et al.* 2002; Hanyga & Seredynska 2005. They conclude that the conventional steady state relationships are not sufficient to characterize the behaviour of two-phase flows in porous media, as they fail to capture the dynamic flow, capillary pressure, temperature effects and interaction of fluid/fluid interfaces arising from various capillary, viscous forces and changes of saturation over prolonged time periods.

In response, Hassanizadeh & Gray (1993) were the first ones to propose the generalized  $P^c$ - $S$  relationships with the inclusion of dynamic capillary pressures. They concluded that dynamic effects do not occur in steady-state flows and as a result, the definition of macroscopic capillary pressure should be based on thermodynamic considerations. The main hypothesis is the dependence of interfaces variables (namely; mass density, temperature, saturation, porosity, etc) and co-existence of phases on Helmholtz free energy. As a result, the generalized  $P^c$ - $S$  relationships with the inclusion of dynamic capillary pressure can be written as,

$$\left( P^{c, dyn} - P^{c, equ} \right) \Big|_s = -\tau \left( \partial S / \partial t \right) \Big|_s \quad (2)$$

where  $\tau$  is the dynamic coefficient,  $\partial S / \partial t$  is the time derivative of saturation,  $P^{c, dyn}$  is the dynamic capillary pressure,  $P^{c, equ}$  is the steady-state capillary pressure and the measurements for all variables is taken at the same saturation value. The dynamic coefficient can be determined from the

slope of Equation 2, which exhibits a linear relationship in form of a straight-line.

As reported in the literature, Equation (2) has been subsequently used by many workers i.e. Theodoropoulou *et al.* (2005), Gielen *et al.* (2005), Dahle *et al.* (2005), Manthey *et al.* (2005), Das & Hassanizadeh (2005); O'Carroll *et al.* (2005); Oung *et al.* (2005); Berentsen *et al.* (2006); Bottero *et al.* (2006); Mirzaei & Das (2007); Das *et al.* (2007) for quantifying the range of the dynamic coefficients  $\tau$  and examining its dependency on the size ( $10^{-3}$ -1m), geometry (2D/3D domains), boundary conditions (entry pressure etc.), physical properties of the porous media (permeability, porosity, etc.), fluid parameters (densities, viscosity ratios etc.), types of heterogeneities (uniform, random or micro-scale), flow characteristics (Newtonian, non-Newtonian etc.) and gravitational effects. Based on the preliminary works of Stauffer (1978), more recently Tzakiroglou *et al.* (2003), Dahle *et al.* (2005), Manthey *et al.* (2005), have proposed upscaling relationships of the form  $\tau = f(\phi, \mu_{nw} / \mu_w, \rho, K, g, \lambda, Ca, P^d)$  where  $\tau$  is the dynamic coefficient,  $\phi$  is the porosity,  $\mu_{nw} / \mu_w$  is the ratio of the viscosities of the non-wetting to wetting phase,  $\rho$  is the density,  $\kappa$  is the permeability tensor,  $g$  is the acceleration due to gravity,  $Ca$  is the dimensionless capillary number,  $\lambda$  and  $P^d$  are Brooks-Corey (1968) parameters. Other state-of-the-art techniques proposed in the literature for quantifying the uncertainty of flows in porous media include the pore-scale modelling techniques developed by Kueper & Frind (1989), Blunt *et al.* (1991), Schroth *et al.* (1998), Nordhaug *et al.* (2003) and Panfilov & Panfilova (2005). Although major efforts have been made to develop upscaling relations based on the quantification of dynamic coefficients and its dependence on various physical parameters, no studies directly report the effects of temperature on dynamic coefficients. The only studies that qualitatively report the effects of temperatures on the two phase porous flow behaviour have been carried out by Sinnokrot *et al.* (1971), Nutt (1981), Hassanizadeh & Gray (1990), Davis (1994), Imhoff (1995), Grant & Salehzadeh (1996), Harr *et al.* (1984), Gatmiri & Dillage (1997), She & Sleep (1998), Narsimhan & Lage (2001), Muralidhar & Shoerey (2003), Grant (2003), Hanyga & Jianfei (2003), and Schembre *et al.* (2006). In the study by Sinnokrot *et al.* (1971), they predict effects of temperature on capillary pressure curves through measurement of drainage and imbibition capillary pressures for three consolidated sandstones and one limestone core. Lo *et al.* (1973) proposed that oil recovery operations are more efficient at higher temperature. They show that the oil relative permeability increases as the residual oil saturation is decreased. They carried out experiments at room temperature and 300°F for Berea sandstone cores. They conclude that the change in relative permeabilities curves is caused by viscosity reductions. Nutt (1981) showed that the displacement of oil by other fluids is affected by capillary bundle size (pore size volume), pore size distribution, interfacial force, interfacial tension, and viscosity ratio. The interfacial force acts as a resistance between two fluids in oil wet system while in water wet system it acts as an addition. Later he shows that at higher temperature faster oil recovery

rates are observed. However, the effects arising from interfacial tensions at high temperature were neglected. Davis (1994) experimentally investigated the effects of temperatures on the Pc-S relationships for water-oil and water-air modes by using a mixture of hydrocarbon oil in two silica sands with different grain sizes. He concluded that the temperature changes have a major effect on the residual wetting and non-wetting phase saturation but have a negligible effect on capillary pressure. In water-oil systems, the residual wetting saturation increases as the temperature increases whilst the residual non-wetting saturation decreases as the temperature increases. He also reported that an increase in temperature also increases the non-wetting to wetting relative permeability ratio, thereby enhancing the fluids movement by reducing the displacement pressures which is a major advantage in oil recovery and water remediation techniques. The reduction of interfacial tension between PCE (Sigma Chemical Co., Milwaukee, WI), and de-ionised and distilled water was measured by Imhoff *et al.* (1995). It was reported that the interfacial tension reduces as the temperature increases between 5°C and 40°C, whilst the kinematic viscosity of water decrease by a factor of 2.3. Grant and Salehzadeh (1996) carried out calculations of several equation models that incorporate the temperature effects on wetting coefficients and capillary pressure functions. They also considered temperature effects on liquid-gas phase interfacial tension and liquid-solid interfacial tension (surface tension). They found that the linear relations of temperature and liquid-gas interfacial tension fit well with the reference interfacial tension data from Harr *et al.* (1984). They noted that the capillary pressure function sensitivity on temperature is mostly due to capillarity. Gatmiri and Delage (1997) later numerically studied a coupled thermo-dynamic flow behaviour of saturated porous media using the finite element method. A mathematical model was developed to deal with thermal variations in saturated porous media. Density variations resulting from temperature changes were modelled through incorporation of bulk modulus and elasticity. They concluded that the variation of permeability tensor in their equation incorporates the effects of temperature changes on dynamic viscosity, thus affecting the capillary pressure-saturation relationships. She and Sleep (1998) studied the temperature dependence of capillary pressure-saturation relationships for water-perchloroethylene (PCE) and water-air systems in silica sand with temperatures ranging from 20°C to 80°C. They reported that for water-PCE system the irreducible water saturation increases and the residual non-wetting saturation decreases as the temperature increases. This result was quite similar to the result of Davis (1994) and Sinnokrot *et al.* (1971) even though they have used different fluid pair (water-CHEVRON 15 white oil) and different sand domain (consolidated natural sandstone). In terms of the capillary pressures, She and Sleep (1998) concluded that capillary pressures decrease when the temperatures increase. However, they show that there are other effects beside interfacial tension and contact angles which can have a significant role in the temperature dependence of capillary pressure-saturation relationships. They used Grant and Salehzadeh's (1996) modified Laplace's equation to determine the capillary pressure functions. Then, by relating Parker and

Lenhard's (1987) hysteretic Pc-Sw relationships with equations from Grant and Salehzadeh (1996), temperature dependence was qualitatively established. Narasimhan and Lage (2001) investigated temperature dependency on viscosity and hence on the global pressure drop of flowing fluid in porous media. They showed that with an increase in temperature the viscosity and the global pressure drop across the domain decrease. Muralidhar and Sheorey (2003) investigated the displacement of oil and the saturation pattern which lead to viscous fingering under isothermal and non-isothermal water flow conditions. Investigations were carried out for both homogenous and heterogeneous domains with high and low permeability values with water injection temperatures of 50°C and 100°C. They conclude that there are three forms that can occur in the presence of both viscous and capillary forces; stable displacement, viscous fingering and capillary fingering and the fact that higher temperature affects the water saturation in the reservoir and reduces the capillary pressure. They show that the oil-water flow has a strong dependency on the permeability distribution. More recently, Grant (2003) has proposed a modified mathematical model that takes into account the effects of temperature on capillary pressure-saturation relationships in homogeneous and heterogeneous porous media by using one parameter and two parameter models. Grant's models are modified forms of the Van Genuchten (1980) equation and one parameter equation model presented by Grant and Salehzadeh (1996). His model takes into account the interfacial tension as a function of temperature. He estimated that the application of one parameter model for water-air system can describe well the temperature effects for water-oil system. However, the two parameter model is better than the one parameter model for a system with a larger temperature range. Grant verified his extended model with temperatures ranging between 273.16K - 448K. Hanyga and Jianfei (2003) investigated the dependency of thermal effects on immiscible two phase flow; and implicitly stated that the capillary pressure-saturation relationships with thermodynamic consideration in non-isothermal systems are significantly different with the same relationships in isothermal systems. Schembre et al., (2006) carried out experiments that predicted the relative permeability of heavy-oil in-situ aqueous phase saturation phase profiles during high temperature imbibition. In their study, they compared experimental data with the simulated results and used two different non-wetting phases. They carried out experiments at 120°C and 180°C. Their results showed that the oil saturation and the water relative permeability decrease when the temperatures increase, resulting in a decrease in capillary pressure.

As it can be inferred from the studies reported above no information concerning the effects of temperature dependency on the measurement of time relaxation factors  $\tau$  can be obtained. The major concern of this work is to therefore investigate the implications of temperature dependency to characterize dynamic coefficients for the PCE-water in the drainage process and hence, the capillary pressure-saturation relations. These effects have been incorporated through the use of empirical relations for fluid and material properties (interfacial tension, residual saturation, viscosity, density, relative permeabilities, etc.) as a function of temperature. Results presented in this article

correspond to a temperature of 40°C for two different materials namely coarse and fine sands.

## MATHEMATICAL MODEL EQUATIONS

The governing equations of the two-phase porous media flow model comprise of the momentum balance (Muskat & Meres, 1936; Demond & Roberts, 1987) and the continuity equations used for modelling two-phase porous media hydrodynamics. In conjunction with the momentum balance equations constitutive relations are required for modelling the material parameters such as the porosity, tortuosity, compressibility, and the particle density (Marshall & Holmes 1973; Farouki 1986; Mandal & Divshikar 1995; Kozak & Ahuja 2005). These properties are independent of any temperature variations. However, fluid parameters such as (water/oil) densities, (water/oil) viscosities, water residual saturation, and liquid-gas/liquid-liquid interfacial tension are assumed to be temperature variant. As such the additional constitutive relations that model the temperature effects are required and can be referred to in the works of (Hanspal & Das 2009; Prasetya, MSc. Thesis UMIST 2007).

## MODELLING METHODOLOGY & RESULTS

### 1. STOMP Simulator

The two phase flow i.e. "water-oil" simulations in this work have been carried out using the "Subsurface Transport Over Multiple Phases" (STOMP) (<http://stomp.pnl.gov/>) simulator (White & Oostrom, 2006) written in FORTRAN. The code has been previously validated against a range of engineering problems which include enhanced oil recovery operations (Scroth *et al.* 1998; Ataie-Ashtiani *et al.* 2001 & 2002; Das *et al.* 2004). The governing equations of the two phase porous flow model are discretized using the Finite Volume technique whilst the temporal discretization procedure follows the Implicit-Theta time-stepping approach. Simulation results were obtained on a computational grid which was refined by increasing the total number of cells by 25%, and no major differences were observed. Convergence was achieved by altering the maximum Newton-Raphson iteration between 16 and 50, and by applying a tolerance value of  $10^{-6}$ . Results indicate that grid refinement has negligible effect on the final capillary pressure-saturation curves. A maximum time step of 600s and time acceleration factor 1.125 have been chosen to yield stable solutions.

### 2. Computation of the Dynamic Co-efficient(s)

Quasi-static & dynamic simulation procedures (Hanspal & Das, 2009) are used for carrying out the simulations until the residual saturations are achieved. To carry out the final integration, an in-house FORTRAN code which performs volume averaging [refer Das *et al.* (2007), Mirzaei & Das (2007)] to determine saturation weighted-average of capillary pressure is used. Damping coefficient ( $\tau$ ) can be determined by using equation (2). For determining the dynamic coefficient knowledge of saturation time derivative data and the capillary pressure data under dynamic and steady-state conditions is post-processed from the simulation output. Averaged data for ( $P^{c,dyn} - P^{c,eq}$ ) and ( $\partial S / \partial t$ ) are then fitted on to the straight line by carrying out linear regression analysis.

### 3. Description of Test Cases & Physical Properties

3-D cylindrical domain shown in Figure-1, similar to the lab scale set-up (Mirzaei and Das, 2006) has been used in this work. The diameter of the column is 10 cm whilst the vertical length in Z-direction is 12 cm. The computational grid consists of 4x4x24 cells with 416 nodes. As heterogeneity effects have not been considered the domains used in this work are fully isotropic. Simulations have been carried out at 20°C, 40°C, 60°C, and 80°C for both coarse and fine sands. At any given temperature, four dynamic simulations and one steady-state simulation have been carried out with a view to generate numerically stable and reliable capillary pressure curves.

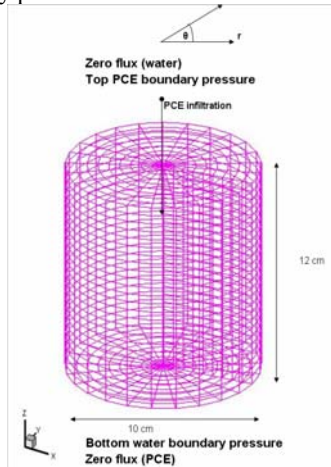


Figure 1: Cylindrical Domain for homogenous porous media

The material properties used in this work correspond to two different sands (coarse & fine sands) and can be referred to in (Hanspal & Das, 2009). Effects of temperature have also been included on the initial and bottom boundary pressures which represent the boundary conditions used in the simulations.

### 4. Boundary Conditions

Simulations represent a pressure cell experiment for drainage process (Ataie-Ashtiani *et al*, 2002 and Mirzaei & Das 2006). Initially, porous media is filled with saturated water and then a fully water saturated porous domain is placed inside the reservoir. The reservoir is filled with oil (PCE). The top boundary condition (BC) is made to have no water flux in the surface by imposing zero flux BC. At each case, the top PCE pressure is kept constant. At the bottom BC, a zero flux BC for PCE and a constant pressure of water is applied. On the side of the cylinder zero flux BC is applied for water and PCE. The pressure gradient and the PCE flow direction is aligned with the gravity direction. The side of the cylinder acts as an impermeable boundary. This is applied so that initially the PCE flow infiltrates in the downward direction. In addition, the initial and bottom boundary conditions for water pressure are defined with consideration to the atmospheric pressure, temperature effects and the gravity forces. At the top face of the porous domain PCE is injected at different pressures for simulating different dynamic cases (Hanspal & Das 2009; Prasetya, MSc. Thesis UMIST 2007).

### 5. Results on Capillary pressure-saturation curves

We present the pressure-saturation curve for four dynamic and one steady-state case for two different materials (i.e. coarse and fine sand at 40°C). Figures 2(a) illustrates the  $P^c$ -S curve for coarse sand at 40°C. The initial capillary pressure is 230 Pa. The dynamic cases exhibit a pressure jump at saturation value 0.39. It can be noticed that the capillary pressure at 40°C is higher than  $P^c$  at 20°C (Hanspal & Das 2009) for the same values of saturation. In figure 2(b) values of  $\partial P^c$  range between 94.7Pa - 232Pa corresponding to the saturation values of 0.394 and 0.217 respectively. The slope gradually increases for lower saturation values

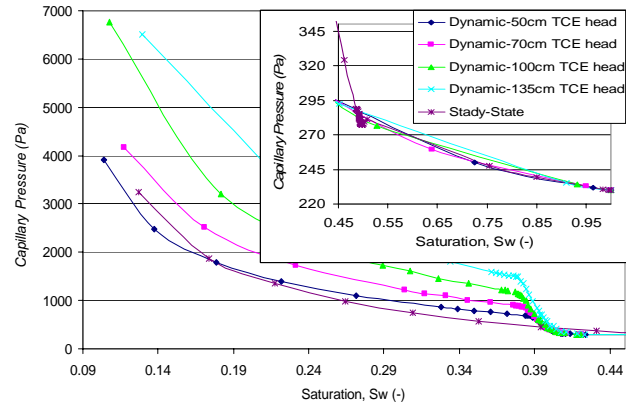


Figure 2(a):  $P_c$ -S curves for Coarse Sand at 40°C

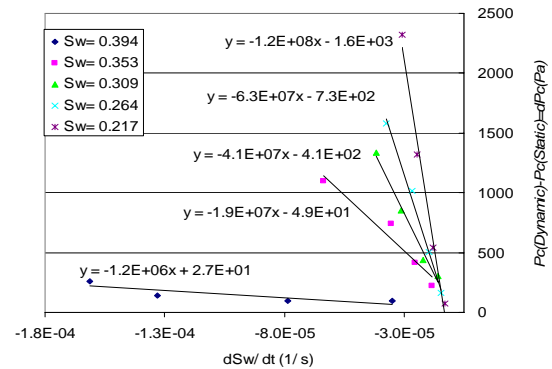


Figure 2(b):  $\tau$  function for Coarse Sand at 40°C

Saturation time derivatives range between  $(-1.61 \times 10^{-04}/s)$  to  $(-1.27 \times 10^{-05}/s)$  whilst the dynamic coefficient ranges between  $1.2 \times 10^{06}$  Pa.s to  $1.2 \times 10^{08}$  Pa.s for the same saturation values. The dynamic coefficient increases whilst  $\partial S / \partial t$  are getting smaller as the saturation decreases near to the residual saturation. The  $R^2$  values vary between 0.74 and 1 which means that at 40°C for the chosen saturations the relations of  $(\partial S / \partial t)$  to  $\partial P^c$  is non-linear. Figure 3(a) illustrates the  $P^c$ -S curves for fine sand at 40°C where the initial  $P_c$  is 823 Pa.  $P^c$  for each case starts increasing rapidly from saturations of 0.356 until the residual saturations are achieved. This occurs between 9-20 hours after the PCE pressure is injected.

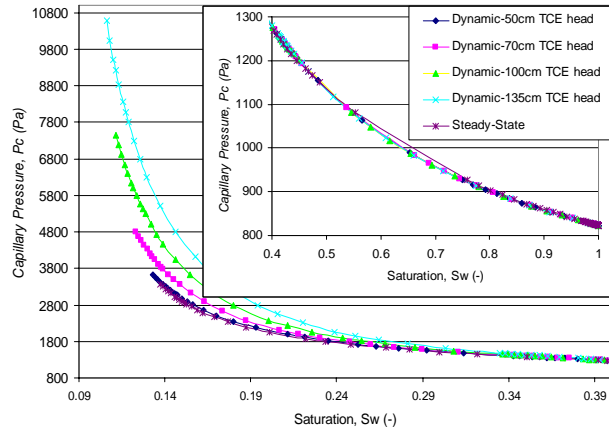


Figure 3(a):  $P_c$ - $S$  curves for Fine Sand at 40°C

This occurs between 9-20 hours after the PCE pressure is injected. Again in this case, no pressure jump occurs in any of cases. The  $P^c$  difference amongst difference PCE pressure cases is higher than the  $P^c$  difference at 20°C. This trend observed for the  $P^c$ - $S$  relationships at 40°C is very similar to the relationships at 20°C (Hanspal & Das, 2009). In Figure 3(b), the values of  $\partial P^c$  range between 867Pa-1480Pa which correspond to the saturation values of 0.363 and 0.156, respectively. The slope increases for lower saturation values. Saturation time derivatives range between  $-1.29 \times 10^{-5}/s$  to  $-7.06 \times 10^{-5}/s$  whilst the dynamic coefficient ranges from  $1.2 \times 10^8$  Pa.s to  $.45 \times 10^{10}$  Pa.s. The dynamic coefficient increases whilst  $\partial S / \partial t$  values get smaller as the saturation reaches the residual values.  $R^2$  values vary between 0.95 and 1, signifying well exhibited linear relationships between  $\partial P^c$  and  $\partial S / \partial t$  at 40°C.

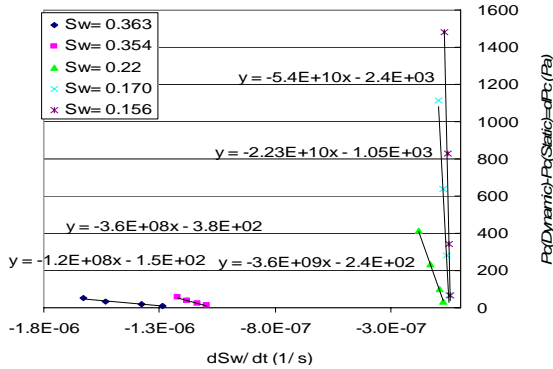


Figure 3(b):  $\tau$  function for Fine Sand at 40°C

Tables 1 & 2 illustrate the computed values of the dynamic coefficients for coarse and fine sands at 40°C.

Sw	$\tau$ (Pa s)	$R^2$
$3.94 \times 10^{-1}$	$1.20 \times 10^6$	0.74
$3.53 \times 10^{-1}$	$1.90 \times 10^7$	0.94
$3.09 \times 10^{-1}$	$4.10 \times 10^7$	0.99
$2.64 \times 10^{-1}$	$6.30 \times 10^7$	1
$2.17 \times 10^{-1}$	$1.204 \times 10^8$	0.99

In general, dynamic coefficients for fine sands are higher than the dynamic coefficients for coarse sand.

Sw	$\tau$ (Pa s)	$R^2$
$3.63 \times 10^{-1}$	$1.20 \times 10^8$	0.98
$3.54 \times 10^{-1}$	$3.60 \times 10^8$	0.98
$2.20 \times 10^{-1}$	$3.60 \times 10^9$	1
$1.70 \times 10^{-1}$	$2.23 \times 10^{10}$	0.992
$1.56 \times 10^{-1}$	$5.45 \times 10^{10}$	0.8

The elevated temperature causes a higher capillary pressure and smaller time derivative of the saturation for the same saturation. In addition, the dynamic coefficients at higher temperatures are higher than their values at lower temperatures for same values of water saturation. These trends are more significant after a critical saturation (low saturations near the residual saturation) at each temperature. The  $R^2$  values show that the data in some cases may not be linear. This is more significant in the case of fine sand domain where the displacement process is very slow and the effects of difference in injection pressure are not as significant as in the coarse sand.

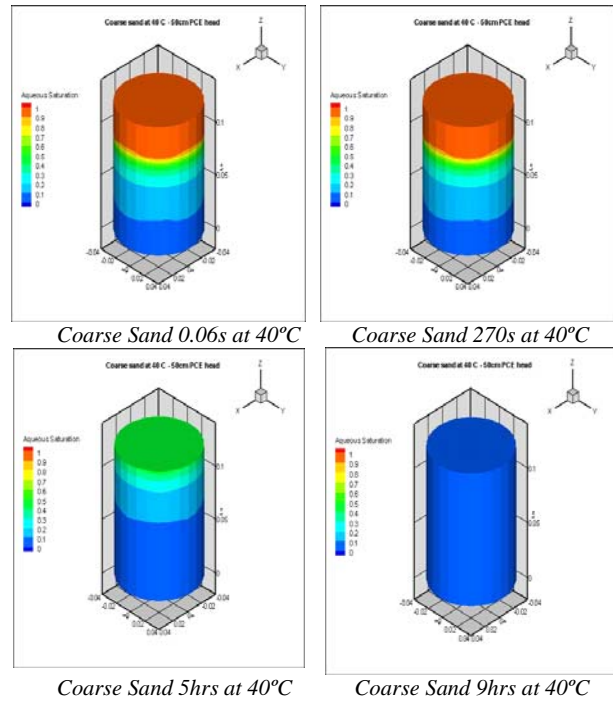


Figure 5: Coarse Sand, Aqueous Saturation @ 40°C

The 3-D saturation plots presented in figures 4 and 5 correspond to the aqueous phase saturation values for coarse and fine sands at 40°C respectively. These figures illustrate the times required to attain the residual saturation at 40°C for coarse and fine sands under dynamic conditions. As can be observed in figure 4 the effects of temperature dominantly occur at earlier time step i.e. 0.06-270.0s until 1 hour, when sudden displacements take place. Then, the displacements get much slower which is marked by a slower decrease in water saturation. At 270.0s (40 °C) PCE

displaces a lot of water at the bottom of the porous domain. Our simulations (Hanspal & Das, 2009) reflect that when the temperature is increased to 80°C, water amount that is displaced in the first 30.0-60.0s decreases. In addition, the effect of gravity and viscous forces along with low water pressure may play an important role to slow the displacement as the temperature increases. The water displacement is not distributed evenly at each node in the cylinder domain. First, the water content in the bottom is displaced, then the displacement is going upward with water in the side of domain is displaced earlier than water in the middle of the domain. The total time required for the full displacement of water in case of coarse sand is 9 hours. However in case of fine sand the times required to attain the residual saturation are much longer. This slower movement of fluids and slower displacement process is observed only in the case of fine sands. High capillary pressures and lower Darcy's velocity is observed because the infiltrate fluids (PCE) need more time to reach the entry pressure.

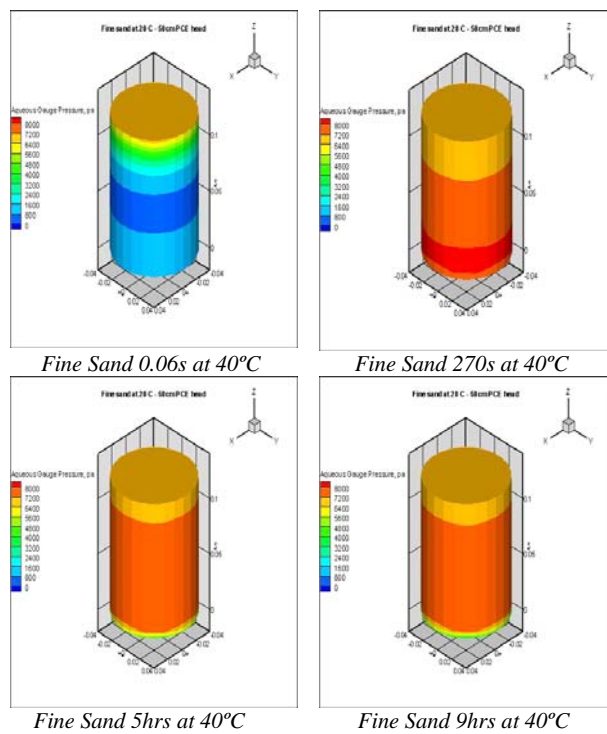


Figure 5: Fine Sand, Aqueous Saturation @ 40°C

Once PCE attains the entry pressure it starts to infiltrate. More over, a much lower permeability in fine sand acts as a resistance to the fluids movement whilst the capillary pressure is very high. This results in high capillary pressure and longer times for PCE to displace water. The total time required for the absolute displacement of water corresponds to 975 hours. The simulated results are very similar to the experimental results obtained by Mirzaei and Das, 2006. We have also observed that with an increment in temperature the dynamic coefficients increase, and hence, more times are required to reduce the saturation or saturation time derivatives decrease. In addition, the range of the dynamic coefficients computed in our studies are relatively higher as reported from the previous studies,

specifically in fine sand domain. The effects of temperature may not be defined as an effect of one or two parameters alone but as the lumped effect of the related parameters (e.g., fluid/ fluid interfacial tension, fluid properties, material properties, and fluid residual saturation). In regards to oil recovery, a slow motion of fluid displacement may decrease the amount or the flow rates for oil recovery, since the residual oil saturations increase, times for recovering oil may be reduced.

## CONCLUSIONS

Simulations have been carried out using STOMP 4.0 to quantify the effects of temperature and fluid properties on the dynamic capillary pressure and in turn on dynamic coefficients for two-phase porous flow in the cylindrical domain. Series of runs were carried out within the range of 20°C-80°C for two different materials (coarse and fine sands) under dynamic conditions to determine the values of dynamic coefficients. The dynamic coefficients found in this work are non linear function of saturation and temperature. This is contrary to the result by Stauffer (1978) which suggests that the dynamic coefficient is independent of saturation. Our results are consistent with most of the recent studies by (Hassanizadeh et al, 2002; Mantney et al, 2005; O'Carroll et al, 2005; Mirzaei and Das, 2006), however the temperature effects as reported in this work have not been reported before. We observe that with an increase in temperature the dynamic coefficients increase and at any given saturation value large time scales are required for non-aqueous phase flow (NAPL) displacements.

## ACKNOWLEDGEMENTS

The authors wish to thank the EPSRC UK for providing funds which enabled this work. Mr. Budi Prasetya an MSc graduate from UMIST is also acknowledged for providing help with post-processing issues.

## AUTHORS BIOGRAPHY

*Dr Navraj Hanspal* is currently a lecturer in the Energy, Environment and Climate Change Group at the University of Manchester. He obtained his Bachelors in Chemical Engineering (2001) from India and later graduated with a PhD in Computational Fluid Dynamics from Loughborough University UK (2005), specialising in mathematical modelling and finite element methods. His current research interests include carbon capture and storage issues, coupled free-porous flows used in a variety of engineering applications, shallow water/sub-surface hydrodynamics and catastrophe/risk modelling all focussing on problems concerning climate change and environmental risk.

*Dr Diganta Bhushan Das* is currently a lecturer in the Advanced Separation Technologies Group at Loughborough University. Prior to this he was a faculty member at University of Oxford UK, and a post doctoral researcher at TU Delft and Princeton universities specialising in Multiphase Flows in Porous Media. His current research interests include bone-tissue engineering, drug delivery techniques and coupled free-porous flows.

## REFERENCES

- Ataie-Ashtiani, B., Hassanizadeh, S.M., Oostrom, M., Celia, M.A., White, M.D., 2001. *Journal of Contaminant Hydrology* 49, 87-109.
- Ataie-Ashtiani, B., Hassanizadeh, S.M., Celia, M.A., 2002. *Journal of Contaminant Hydrology* 56, 175-192.
- Ataie-Ashtiani, B., Hassanizadeh, S.M., Oung, O., Westrate, F.A., Bezuijen, A., 2003. *Environmental Modelling & Software* 18, pp 231-241.
- Bear, J., Verruijt, A. 1972. *Modelling Groundwater Flow & Pollution, Theory and Applications of Transport in Porous Media*. Boston, MA: Reidel, 1987
- Beliaev, A.Y., Hassanizadeh, S.M., 2001. *Journal of Transport in Porous Media* 43, 487-510.
- Beliaev, A.Y., Schotting, R.J., 2001. *Computational Geosciences* 5, 345-368.
- Berentsen, C.W.J., Hassanizadeh, S.M., Bezuijen, A., Oung, O., 2006. *Proceedings of the XVI International Conference on Computational Methods in Water Resources (CMWR)*, Copenhagen, Denmark
- Blunt MJ, King P. 1991. *Transport in Porous Media*, 6(4):407-33.
- Brooks, R.H., Corey, A.T., 1964. *Hydrology Papers*, Colorado State University
- Dahle, H.K., Celia, M.A., Hassanizadeh, S.M., 2005. *Transport in porous Media* 56, 329-350
- Das, D.B., Hassanizadeh, S.M., 2005. *Upscaling Multiphase Flow in Porous Media: From Pore to Core and Beyond*. Springer, Berlin pp 1-3, ISBN: 1-4020-3513-6
- Das, D.B., Hassanizadeh, S.M., Rotter, B.E., Ataie-Ashtiani, B., 2004. *Transport in Porous Media* 56, 329-350.
- Das, D.B., Mirzaei, M., Widdows, N., 2006. *Journal of Chemical Engineering Science* 61, 6786-6803.
- Das, D.B., Gaudie, R., Mirzaei, M., 2007. *AIChE Journal*
- Davis, E.L., 1994. *Journal of Contaminant Hydrology* 16, 55-86.
- Demond, A.H., Roberts, P.V., 1987. *American Water Resources Bulletin*.
- Farouki, T.O., *Thermal properties of soil*, 1986. *Trans Tech Publications*, Clausthal-Zellerfeld, Germany, pp 29-30.
- Gatmiri, B., Delage, P., 1997. *International Journal for Numerical and Analytical Methods in Geomechanics* 21, 199-225.
- Geilen A.J.M., Hassanizadeh, S.M., Nordhaug, H.F., Leijmse A., 2005. *Special Issue on: Upscaling Multiphase Flow in Porous Media: From Pore to Core and Beyond*. Springer, The Netherlands
- Grant, S.A., 2003. *Water Resources Research* 39(1).
- Grant, S.A., Salehzadeh, A., 1996. *Water Resources Research*, 32(2), 261-270
- Haines W.B., 1930. *Journal of Agricultural Science* 20, 97-116
- Hanyga, A., Jianfei, L., 2004. *International Journal of Engineering Science* 42, 291-301.
- Hanyga, A., Seredynska, M., 2005. *Transport in Porous Media* 59, 294-265.
- Hassanizadeh, S.M., Gray, W.G., 1990. *Advances in Water Resources* 13(4).
- Hassanizadeh, S.M., Gray, W.G., 1993. *Water Resources Research* 29 (10), 3389-3405.
- Hassanizadeh, S.M., Celia, M.A., Dahle, H.K., 2002. *Agricultural Sciences* 7(2), 69-71
- Helmig, R., 1997. *Multiphase flow and transport processes in the subsurface*. Springer, Berlin. 367pp.
- Imhoff, P.T., Frizzell, A., Miller, C.T., 1997. *Environmental Science and Technology* 31, 1615-1622.
- Kueper, B.H., Frind, E.O., 1989. *Journal of Contaminant Hydrology* 5, 83-95.
- Kozak, J.A., Ahuja, L.R., 2005. *Soil Science Society*.
- Kovscek, A.R., 2003. *Quarterly Technical Progress Report*, DE-FC26-00BC15311.
- Mandal, J.N., Divshikar, D.G., 1995. *Soil testing in civil engineering*. A.A Balkema Publisher, Brookfield, USA, pp.10-90.
- Manthey, S., Hassanizadeh, S.M., 2005. *Transport in Porous Media* 58, 121-145.
- Marshall, T.J., Holmes, J.W., 1973. *Soil Physics*. Cambridge University Press
- Meyer, C. A., McIntock, R. B., Silvestri, G. J., Spencer Jr, R. C., 1967. *ASME steam tables: Thermodynamic and transport for steam and water*, pp 13-30.
- Mirzaei, M., Das, D.B., 2007. *Chemical Engineering Science* 62, 1927-1947.
- Muralidhar, K., Sheorey, T., 2003. *International Journal of Thermal Sciences* 42, 665-676
- Murdoch, A.I., Hassanizadeh, S.M., 2002. *International Journal of Multiphase Flow* 28, 1091-1123
- Muskat, M., Mears, M., 1936. *Physics* 7, 346-363.
- Narasimhan, A., Lage, J.L., 2001. *Journal of Heat Transfer* 123.
- Nordhaug HF, Celia M, Dahle HK. *Advances in Water Resources* 2003; 26(10):1061-1074.
- Nichols, W.E., Aimo, N.J., Oostrom, M., White, M.D., 1997. *STOMP application guide*. PNNL-11216, UC-2010.
- Nutt, C.W., 1981. *Proceeding of The Royal Society of London. Series A, Mathematical and Physical Science* 382, pp. 155-178.
- O'Carroll, D.M., Phelan, T.J., Abriola, L.M., 2005. *Water Resources Research* 41
- Oostrom, M., Meck, D.H., White, M.D., 2003. *STOMP an introductory short course*. Pacific Northwest National Laboratory, Richland, Washington.
- Oung, O., Hassanizadeh, S.M., Bezuijen, A., 2005. *Journal of Porous Media* 8(3), 247-257
- Panfilov M, Panfilova I. 2005. *Transport in Porous Media* 2005; 58(1-2):87-119.
- Reid, R. C., Prausnitz, J. M., Poling, B. E., 1987. *Mcgraw Hill, Inc.* pp 433-485.
- Schembre, J.M., Kovscek, A.R., 2005. *Journal of Energy Resources* 127.
- Schembre, J.M., Kovscek, A.R., 2006. *Transport in Porous Media* 65: 31-51.
- Schembre, J.M., Tang, G.-Q., Kovscek, A.R., 2006. *SPE 938831 (Society of Petroleum Engineers)*.
- Schroth, M.H., Istok, J.D., Selker, J.S., Oostrom, M., White, M.D., 1998. *Advances in Water Research* 22 (2), 169-183
- She, H.Y., Sleep, B.E., 1998. *Water Resources Research* 34, no10 pp2587-2597.
- Sinnokrot, A.A., Ramey Jr, H.J., Marsden Jr, S.S., 1971. *Society of Petroleum Engineers (SPE) Journal*, 11, 13-22



Stauffer F., 1979 Proceedings of the IAHR conference on scale effects in porous media, Thessaloniki, Greece.

Theodoropoulou, M.A., Sygouni, V., Karoutsos, V., Tsakiroglou, CD 2005. International Journal of Multiphase Flow 31 (10-11), 1155-1180

Tzakioglou CD, Theodoropoulou MA, Karoutsos V. Nonequilibrium, 2003 AIChE Journal 49(10):2472-2486.

White, M.D., Oostrom, M., 2000. STOMP 2.0 theory guide. PNNL-12030, UC-2010.

White, M.D., Oostrom, M., 2006. STOMP 4.0 user guide. PNNL-17782.