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# Pore2Field - Flows and Mechanics in Natural Porous Media from Pore to Field Scale

Pore2Field - Physique des écoulements en milieux poreux naturels : de l'échelle du pore à l'échelle du réservoir

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Pore2Field – Flows and Mechanics in Natural Porous Media from Pore to Field Scale Pore2Field – Physique des écoulements en milieux poreux naturels : de l'échelle du pore à l'échelle du réservoir

# Steady-State Two-Phase Flow in Porous Media: Review of Progress in the Development of the *DeProF* Theory Bridging Pore to Statistical Thermodynamics Scales

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**Résumé** — Écoulement diphasique stationnaire en milieu poreux : revue des avancées sur les développements de la théorie *DeProF* reliant l'échelle du pore à l'échelle de la thermodynamique statistique — Cet article présente les efforts de recherche effectués au travers d'une étude expérimentale, d'une analyse théorique et d'une modélisation, afin de développer une théorie complète pour les écoulements diphasiques stationnaires en milieu poreux (théorie *DeProF*). Les dernières avancées sont mises en avant et les problématiques restées ouvertes sont exposées.

Les premières tentatives dans ce domaine remontent aux années 80, avec l'analyse, la description et la modélisation des phénomènes régissant les écoulements diphasiques à l'échelle du pore. Des simulateurs appropriés à l'échelle de centaines et/ou de milliers de pores (échelle du réseau) ont été développés dans les années 90. Parallèlement, des recherches expérimentales approfondies ont permis d'identifier trois mécanismes d'écoulements élémentaires pour représenter l'écoulement moyen à l'échelle macroscopique : l'écoulement à travers la fraction d'huile connectée, la dynamique des globules d'huile et l'écoulement par circulation de gouttes et d'établir leur contribution relative dans l'écoulement macroscopique.

Les efforts faits pour apporter une interprétation physique cohérente aux observations expérimentales, c'est-à-dire pour réaliser la cartographie des régimes d'écoulement, ont jeté les bases de ce qui est devenu la théorie de la décomposition en écoulements élémentaires (*DeProF*). Parmi les principaux résultats/ caractéristiques de la théorie *DeProF*, on compte l'identification des paramètres du système et la définition, dans le respect des principes de l'ergodicité, du domaine des différentes combinaisons d'écoulement physiquement admissibles pouvant représenter l'écoulement macroscopique moyen.

L'utilisation, comme outil de simulation, de ce modèle mécanistique (années 2000) a permis de découvrir de nombreuses propriétés caractéristiques du processus étudié. On notera l'importance de l'existence, dans le domaine des paramètres de fonctionnement du processus, d'une fenêtre d'intérêt optimale sous la forme d'une surface lisse et continue. La justification de l'existence de conditions opératoires optimales pour le transport de l'huile, dissimulées dans l'utilisation des courbes de perméabilité relatives, a récemment été apportée par la théorie *DeProF*. Les efforts de recherche se poursuivent actuellement (années 2010) pour élaborer une approche physique s'appuyant sur la thermodynamique statistique et sur le concept *aSaPP* "aussi spontané que physiquement possible" (*as Spontaneous as Physically Possible*), qui confirme la corrélation entre l'efficacité du transport et la multiplicité des combinaisons d'écoulements élémentaires.

Abstract — Steady-State Two-Phase Flow in Porous Media: Review of Progress in the Development of the DeProF Theory Bridging Pore to Statistical Thermodynamics Scales — Scope of present article is to present the research efforts (implementing experimental study, theoretical analysis and modeling) taken towards the development of a complete theory for steady-state concurrent two-phase flow in porous media (the DeProF theory). The current state of progress is outlined and open problems are addressed. First attempts are traced back in the 1980s with the analysis, description and modeling of phenomena governing two-phase flow in pore scale. Appropriate simulators extending over hundreds and/or thousands of pores (network scale) were developed in the following decade (1990s); in parallel, extensive experimental research work identified three prototype/elementary flows comprising the average macroscopic flow, namely connected-oil pathway flow, ganglion dynamics and drop traffic flow and mapped their relative contribution to the macroscopic flow in terms of the process parameters.

Efforts to provide a consistent physical rationale to explain the experimental observations, i.e. the map of prototype flow regimes, laid the grounds for developing the DeProF (Decomposition in Prototype Flows) theory. Amongst the main results/features of the DeProF theory was the identification of the actual operational and system parameters of the process and the introduction – according to ergodicity principles – of the domain of physically admissible internal flow arrangements of the average macroscopic flow.

Use of the respective mechanistic model as a simulation tool (in the 2000s) revealed many characteristic properties of the sought process. Important is the existence of optimum operating conditions in the form of a smooth and continuous locus in the domain of the process operational parameters. This characteristic remained in latency within the relative permeability curves, until recently unveiled by the DeProF theory. Research efforts continue in the present (2010s) by elaborating appropriate physical considerations based on statistical thermodynamics and the introduction of the aSaPP (as Spontaneous as Physically Possible) concept that corroborates the correlation of the process efficiency to the multiplicity of the internal flow arrangements.

# NOTATION

- A tilde embelishment indicates a dimensional variable No tilde embelishment denotes a dimensionless
- variable Ca Capillary number
- Co Coalescence factor between oil ganglia
- Energy utilization coefficient  $f_{\rm EU}$
- Coefficient of oil fragmentation  $f_{\rm OF}$
- k Absolute permeability of the porous medium

Boltzman type constant quantity to be derived in k<sub>DeProF</sub> accordance with the DeProF theory on SS2qFPM

- Actual number of different mesoscopic flow arrange- $N_{\rm PAS}$ ments (reduced per unit volume of porous medium) consistent with the macroscopic flow at (Ca, r)
- $\widetilde{p}$ Macroscopic pressure
- r Oil/water flowrate ratio
- Wetting phase saturation
- Oil flowrate
- Water flowrate
- Superficial velocity of water
- $S_w \ \widetilde{q}_o \ \widetilde{q}_w \ \widetilde{U}_w \ \widetilde{U}_o$ Superficial velocity of oil
- $U_{ow}^{DOF}$ Reduced superficial velocity of o/w interfaces through disconnected oil flow

Reduced macroscopic pressure gradient x

Vector containing the geometrical and topological X<sub>p.m.</sub> parameters of the pore network

 $\tilde{z}$ Macroscopic flow direction

### Greek letters

- β Porous medium volume fraction occupied by the connected oil
- $\widetilde{\gamma}_{ow}$ Oil-water interfacial tension
- $\theta^0_A$ Static contact angle for advancing oil-wate meniscus
- $\theta_R^0$ Static contact angle for receding oil-water meniscus
- к Oil/water viscosity ratio
- $\tilde{\mu}_o$ Dynamic viscosity of oil
- Dynamic viscosity of water  $\widetilde{\mu}_w$
- $\xi_{ow}^D$ Contribution of droplets in the transfer of o/w interface in two-phase flows
- Ф' Any physically admissible quantity (a prime denotes a physically admissible quantity)
- Φ Expected mean macroscopic flow quantity, corresponding to the ensemble of  $\Phi$ '
- ω Fraction of all the ganglion cells over all the DOF region cells
- Measure of the degrees of freedom of the process at  $\Omega_{PAS}$ the mesoscopic scale

### Abbreviations

aSaPP	As Spontaneous as Physically Possible
CPF	Connected Pathway Flow
DeProF	Decomposition in Prototype Flows
DOF	Disconnected Oil Flow
DTF	Drop Traffic Flow
EMT	Effective Medium Theory
EOR	Enhanced Oil Recovery
FAV	Flow Arrangement Variables
GD	Ganglion Dynamics
LGD	Large Ganglion Dynamics
OOC	Optimum Operating Conditions
PAS	Physically Admissible Solution(s)
PBE	Population Balance Equation(s)
p.u.v.p.m.	per unit volume of porous-medium
SGD	Small Ganglion Dynamics
SS2φF	Steady-State two-phase Flow
$SS2\phi FPM$	Steady-State two-phase Flow in Porous Media
2φFPM	Two-phase Flow in Porous Media

## **INTRODUCTION**

# The Physical Process: Steady-State Two-Phase Flow in Porous Media (SS2 $\phi\text{FPM}$ )

Two-phase Flow in Porous Media ( $2\varphi$ FPM) occupies a central position in physically important processes with practical applications of industrial and environmental interest. Some examples are (Tsakiroglou *et al.*, 2007):

- the oil and gas production from underground reservoirs;
- the groundwater and soil contamination by organic compounds and relevant methods of subsurface restoration;
- the operation of multiphase trickle-bed reactors;
- the drying of hygroscopic capillary porous media;
- the gas/water flow and transport in the cathode of proton exchange membrane fuel cells.

Addressing the new challenges of the 21st century, such as climate change, environmental impacts, energy diversification and water resource management, research has been stepped up in a variety of fields, including the geological storage of  $CO_2$ , the production of shale gas and tight gas reservoirs and Enhanced Oil Recovery (EOR) processes. A better understanding of flows and related physical processes is essential to effectively tackle these topics and come up with appropriate technical solutions. To achieve this, it is necessary to consider different scales, from the pore scale (micrometers) to the field scale (hundreds of meters). One of the major difficulties

involved is effectively grasping the coupling between different scales and related physical phenomena. Processes that occur on a microscopic scale determine mechanical and flow behaviors on a larger scale. In addition, a coarser description is necessary on a large scale due to a lack of detailed knowledge of the field and the need to keep computational costs down. What makes the problem challenging is the need for an unified description linking the different scales and the physics involved. While characterization and modeling on different scales are giving rise to active and promising theoretical, experimental and numerical research, there is still a need to improve integration of all the relevant scales and the associated physical phenomena at an early stage (IFP Energies nouvelles, 2011).

The scope of this paper is:

- to present the research efforts comprising experimental study, theoretical analysis and modeling – towards the development of a new theory for Steady-State Two-Phase Flow In Porous Media (SS2φFPM), namely the *DeProF* theory;
- to outline the current state of progress in the development and evolution of the particular theory;
- to identify the open problems yet to be addressed.

Why would a theory on steady-state be of any value? The majority of the industrial applications of two-phase flow in porous media are based on inherently transient (non-stationary) processes, classified into capillary fingering, viscous fingering and stable front displacement. In addition, the medium where the process takes place is generally macroscopically heterogeneous. To tackle the problem and understand the physics of general two-phase flow in porous media in a broader context, there is need to understand first the stationary case, *i.e.* steady-state flow in a macroscopically homogeneous medium. Two-phase flow in porous media is a dissipative process, therefore, an external energy input balances the internal energy losses to maintain it at any certain equilibrium. Steady-state two-phase flow in porous media is a process in statistical equilibrium, in the sense that average flow properties and distribution functions are invariant in time. As it will be shown in Section 2, the last two sentences are absolutely fundamental in understanding the sought process and provide the keys for deciphering the underlying physical mechanisms.

Is steady-state conveniently susceptible of analysis and modeling? Albeit simple, steady-state  $2\varphi$  flow in porous media, like many physical and physicochemical processes of practical interest, does not yield to "one-shot" theoretical analysis and modeling. This intransigence is due to the following causes. First, the vast magnitude of the computational effort that "one-shot" modeling/simulation would require. Second, the fact that the process itself may be affected strongly by factors residing at several different length and/or occurring over widely different time scales. In such cases a rational and cost effective (not to say "the only feasible") approach is hierarchical theoretical modeling (Payatakes *et al.*, 1998). The *DeProF* theory for SS2φFPM implements hierarchical theoretical modeling across the following stages:

- pore-scale models;
- Disconnected Oil Flow (DOF) (Ganglion Dynamics and Drop Traffic Flow) models;
- decomposition of the macroscopic flow in a "base" of three prototype flows;
- micro-to-macro consistency balances;
- determination of the canonical ensemble of admissible mixtures of prototype flows (the physically admissible flow patterns);
- examination of the statistical thermodynamics aspects of the process.

The paper deploys in three directions: in the next section, there is a brief recount of the *DeProF* theory precursor works (in order to reveal how an intercommunicating and balanced mixing of experimental study and theoretical analysis and modeling can leverage the development of a robust theory); then, the paper will continue with a presentation of the basic aspects of the *DeProF* theory and its main findings; in the last section, there will be a presentation of the recent progress made in the conceptual justification of the main *DeProF* theory findings; the paper will finally conclude with a listing of the main results and characteristics of the proposed theory and open problems that still needs to be addressed.

#### Brief Recount of the DeProF Theory Evolution

The time- and scale-wise evolution of research efforts, actually comprising a research program leading to the development of the *DeProF* theory for steady-state  $2\varphi$  flow in porous media, is depicted in Figure 1. The reader may wish to skip this passage and continue reading in Section 1.

#### The Precursor Works - Early Period

In the early 1980s, Payatakes et al. (1981) presented a simulation method to predict the fate of solitary ganglia (small disconnected oil blobs occupying one to a few pores) during immiscible displacement in water-wet unconsolidated granular porous media. For each ganglion size, hundreds of realizations were performed with random ganglia shapes in a  $100 \times 200$  planar pore network and different porous medium topology, initial size, shape and orientation of the oil ganglion and the capillary number. The Monte Carlo simulations showed that ganglia tend to become aligned to the macroscopic flow direction; another interesting observation was that ganglion breakup remained virtually unaffected whereas stranding decreased markedly with increasing values of the capillary number. The first observation is directly related to the macroscopic observation of the disconnection of the non-wetting (oleic) phase, whereas the second with the observation that even small, stranded oil ganglia have a chance of mobilization. These

observations shaped future research efforts towards modeling ganglia behavior within a flood.

Next year, Payatakes (1982) describes and analyzes all the drainage or imbibition phenomena that regulate oil-bank formation during Enhanced Oil Recovery by chemical flooding. He concentrated on the case where the non-wetting phase is oleic (oil-based) and the wetting phase is aqueous. The local flow conditions, necessary for mobilization/stranding of solitary ganglia to take effect, were analyzed and the solitary ganglion mobilization criterion was derived. Appropriate ganglion Population Balance Equations (PBEs) were furnished in integrodifferential form as a first attempt to model the transport of the disconnected phase (oil) by bridging the micro/mesoscopic scale behavior of ganglia to the macroscopic transport characteristics of the total flow. The PBEs comprise two equations: a balance of moving and a balance of stranded ganglia of all sizes; the two equations are coupled because moving ganglia can generate stranded ones and stranded ones can generate or coalesce with moving ones; the relative intensity of each phenomenon was quantified by appropriate system factors. The PBEs remained unsolved until, a few years later, the system factors were evaluated through network simulations (Constantinides and Payatakes, 1996).

Then, Payatakes and Dias (1984) reviewed the current (at that time) state-of-the-art in modeling two-phase flow in porous media and discussed topics such as porous media, flow regimes displacement in single capillaries and doublets, the modeling of immiscible displacement, the formation of ganglia, the mobilization and quasi-static displacement of ganglia, the dynamic displacement of ganglia, the dynamics of ganglion populations. They concluded with suggestions for future work.

In parallel, Ng and Payatakes (1985) examined the flowrate – pressure drop relation assumed in permeability models and showed that the – by then – contemporary simplifying assumption can deviate quite substantially from reality. Actually, the pressure drop along a unit cell is inversely proportional to its conductance, rather than being proportional to its projected length on the direction of the pressure gradient. These observations underlined the significant yet often overlooked fact that transport phenomena in porous media are strongly affected by the cooperative behavior of a large ensemble of pores (unit cells). This study implicitly advocated the necessity to invest in developing appropriate simulators for two-phase flow in pore networks, since only network analysis can take in account this aspect of transport in permeable media.

For this reason, a theoretical simulator of immiscible displacement of a non-wetting fluid by a wetting one in a random porous medium was developed by Dias and Payatakes (1986a, b). The porous medium was modeled as a network of randomly sized unit cells of the constricted-tube type. Under creeping-flow conditions, the problem was reduced to a Evolution of DeProF theory for Steady-State two-phase Flow in Porous Media (SS2 oFPM) Time- & scale-wise evolution of research leading to the development of the DeProF theory

Monte-Carlo simulation of the fate of solitary oil ganglia during immiscible µ-displacement in porous media Payatakes <i>et al.</i> (1981) Pore-to-mesoscale	Theoretical a	Immiscible u-displacement and Ganglion Dynamics in porous media Payatakes and Dias (1984) Pore-to- mesoscale	ical models Network models for 2φFPM Dias and Payatakes (1986a, b) Mesoscale Motion o solitary o ganglia ir porous mec Hinkley <i>et a</i> (1987)	Theoretical model of collision- coalescence of oil ganglia Constantinides and Payatakes (1991) Pore-scale f il planar a non-pla dia mode vi. networ Avraam a (1994)	Network simulatior of SS2φFP Constantinide and Payataka (1996) Mesoscale in and re dur SS2q ks Avrea Paya (19	Me M S b C M Dyn s S Nur s S Vala N S S Perms ing S FPM m and takes 95)	echanistic Model of S2φFPM aased on Canglion amics (GD) n. solution of PBEs vanides <i>et al.</i> (1998) desoscale Flow regin and relper during S2φFPI strong wettabili Avraam ar Payatakes (1	DeProF mechanistic model SS2φFPM - decomposition in prototype flows Valavanides and Payatakes (1998, 2000, 2001) Pore-to-mesoscale	DeProF prediction of Optimum Operating Conditions (OOC) for SS2\pFPM Valavanides an Payatakes (200 Pore-to-statistic thermodynamic scale	aSaPP conceptual justification of the existence d of OOC in 3) SS2 $\varphi$ FPM valavanides (2010) Statistical thermodynamics Reveal of latent experimental evidence on the existence of OOC for SS2 $\varphi$ FPM valavanides (2010)
1980				1990			2000			2010
# pores: p.m. scales: Study scales:	1 10 Pore Microscale	10 <sup>3</sup>	Me	10 <sup>6</sup> esoscopic	Network /	10 <sup>9</sup> core	3	Macroscopic	Statisti	$+\infty$ Field cal thermodynamics

#### Figure 1

Milestones in the *DeProF* theory evolution spanning three decades. *DeProF* is the apex of the "Payatakes group" research efforts on the study of Steady-State two-phase Flow in Porous Media (SS2 $\varphi$ FPM), combining experimental research, theoretical analysis, numerical simulations and semianalytical and mechanistic modeling.

system of linear equations, the solution of which gives the instantaneous pressures at the nodes and the corresponding flowrates through the unit cells. The pattern and rate of the displacement were obtained by assuming quasi-static flow and taking small time increments. The effects of the capillary number, Ca and the viscosity ratio,  $\kappa$ , were studied. The results confirmed the importance of the capillary number for displacement but they also showed that for moderate and high Ca values the role of the viscosity ratio is pivotal. In addition to the residual saturation of the non-wetting fluid, the simulator predicted the time required for the displacement, the pattern of the transition zone, the size distribution of the entrapped ganglia and the acceptance fraction as functions of Ca, k and the porous-medium geometry. The behavior of non-wetting ganglia undergoing immiscible displacement in a porous medium was also studied with the help of the aforementioned simulator. The fluid of a non-wetting ganglion is in contact with the wetting fluid at menisci which were assumed to be spherical cups. The flow in every constricted unit cell occupied by a single fluid was modelled as flow in a sinusoidal tube. The flow in every unit cell containing a meniscus and portions of both fluids was treated with a combination of a Washburn-type analysis and a lubrication-theory approximation. The flow problem was thus reduced to a system of linear equations the

solution of which gives the instantaneous pressures on the nodes, the flowrates through the unit cells and the velocities of the menisci. The dependence of the average ganglion velocity on ganglion size, capillary number, viscosity ratio and dynamic contact angle was examined for the simple case of motion between straight rows of spheres.

At that same period, fundamental to the study of oil ganglion population dynamics was the experimental study of Hinkley *et al.* (1987) on the motion of solitary oil ganglia. Measurements of ganglion velocity were taken as a function of the capillary number and of the ganglion size for favorable and unfavorable viscosity ratios. This was done in a square bead pack, free from the complication of ganglion breakup. A visual study of ganglion motion was also conducted and the effect of pressure gradient direction on ganglion motion was investigated and two distinct modes of motion of ganglia were observed – quasistatic and dynamic displacements.

Since the problem of collision and coalescence of nonwetting ganglia is central to understanding the mechanics of bank formation during immiscible two-phase flow in porous media, Constantinides and Payatakes (1991) presented a theoretical model of the process of collision and coalescence of a pair of mobilized ganglia in porous media and investigated the conditions under which coalescence is prompt or difficult. The porous medium was modelled as a three-dimensional network of randomly sized unit cells of the constricted-tube type and the problem of simultaneous flow of the two ganglia in the porous medium was solved using the network approach. The details of the flow near and between the two colliding menisci were analyzed with a film drainage model, which took into account the presence of the constraining pore wall, the wetting film which surrounds the ganglia (by occupying roughness features on the pore wall) and the hydrodynamic interactions of the three liquid bodies. The factors controlling film drainage in a single throat were investigated. The model was used to evaluate the probability of coalescence between pairs of colliding ganglia. Using this model, the dependence of the probability of coalescence given a collision, on the parameters that affect the flow (capillary number Ca, viscosity ratio  $\kappa$  and dynamic contact angles) was investigated.

At the same period, a comparative experimental study (Avraam et al., 1994) of steady-state two-phase flow in two types of model porous media was deployed to determine the effects of non-planarity on the flow mechanisms and the mesoscopic flow behavior. The two model porous media had virtually the same pore geometry but one had a planar network skeleton, whereas the other had a nonplanar (two-layer) skeleton. The latter was a new type of model porous medium that permited detailed visual observation and quantitative measurements without sacrificing the 3-D character of the pore network topology. The capillary number and the flowrate ratio were changed systematically, whereas the viscosity ratio and the wettability (contact angle) were kept constant. Conventional relative permeabilities were determined and correlated with the pore-scale flow phenomena. In the range of parameter values investigated, the flow mechanism observed was Ganglion Dynamics (intrinsically unsteady but giving a time-averaged steady-state). The non-planarity has shown to have small qualitative but significant quantitative effects.

Following that, Avraam and Payatakes (1995, 1999) (see also Tsakiroglou et al., 2007) performed a groundbreaking experimental study on the pore-scale flow mechanisms and the relative permeabilities during steady-state two-phase flow in a large model pore network of the chamber-and-throat type, etched in glass. The wetting phase saturation,  $S_w$ , the capillary number, Ca and the viscosity ratio,  $\kappa$ , were changed systematically, whereas the wettability (contact angles,  $\theta_0^R$ ,  $\theta_0^A$ ), the coalescence factor Co and the geometrical and topological parameters were kept constant. The fluid flow rate and the pressure drop were measured independently for each fluid. During each experiment, the pore-scale flow mechanisms were observed and videorecorded and the mean water saturation was determined with image analysis. Four main flow regimes were observed, namely Large Ganglion Dynamics (LGD), Small Ganglion Dynamics (SGD), Drop Traffic Flow (DTF) and Connected Pathway Flow (CPF). The experimental demonstration that LGD, SGD and DTF prevail under flow conditions of practical interest, for which the widely held dogma presumes Connected Pathway Flow, necessitated the drastic modification of that assumption. The relative permeabilities were shown to correlate strongly with the flow regimes. The conventional relative permeabilities and the fractional flow of water, were found to be strong functions not only of the water saturation,  $S_w$ , but also of Ca and  $\kappa$  (with the wettability, the coalescence factor and all the other parameters kept constant).

In parallel, Constantinides and Payatakes (1996) developed a computer-aided simulator of steady-state two-phase flow in consolidated porous media. The porous medium was modelled as a 3-D pore network of suitably shaped and randomly sized unit cells of the constricted-tube type. The problem of two-phase flow was solved using the network approach and the basic models developed by Constantinides and Payatakes (1991) for the collision and coalescence of oil ganglia. The wetting phase saturation, the viscosity ratio, the capillary number and the probability of coalescence between two colliding ganglia were changed systematically, whereas the geometrical and topological characteristics of the porous medium and wettability were kept constant. In the range of the parameter values investigated, the flow behavior observed was ganglion population dynamics (intrinsically unsteady but giving a time-averaged steady-state). The mean ganglion size and fraction of the non-wetting phase in the form of stranded ganglia were studied as functions of the main dimensionless parameters. Fractional flows and relative permeabilities were determined and correlated with flow phenomena at pore level. Effects of  $S_w$ ,  $\kappa$ , Ca and Co on relative permeabilities were examined. With the computer aided simulator, it was then made possible to solve the Population Balance Equations (PBEs). The network simulations produced tabulated results for the values of the system factors contained in the PBEs as a function of the system parameters and water saturation.

Based on the observations/results of the experimental works of Avraam and Payatakes (1995) and Constatinides and Payatakes (1996) that has shown that the pore-scale flow mechanism during steady-state two-phase slow in porous media is Ganglion Dynamics (GD) over a broad and practically significant range of the system parameters, it was a rational decision to develop a mechanistic model of steadystate two-phase flow for those cases where the dominant flow regime is Ganglion Dynamics. The approach was based on the ganglion Population Balance Equations already furnished by Payatakes (1982) in combination with the microflow network simulator of Constantinides and Payatakes (1996). The fundamental information on the cooperative flow behavior of the two fluids at the scale of a few hundred pores was expressed through the system factors, which are functions of the system parameters and were -by that time- calculated using the network simulator. These system factors were utilized in the Population Balance Equations to predict the macroscopic mass transport characteristics of the process. The dependence of the conventional relative permeability coefficients not only on  $S_w$  but also on Ca,  $\kappa$ ,  $(\theta_A^0, \theta_R^0)$ , Co, as well as  $\mathbf{x_{p.m.}}$ , was explained and predicted on a mechanistic basis. Sample calculations have been performed for steady-state fully developed and steady-state non-fully developed flow conditions. The number distributions of the moving and the stranded ganglia, the mean ganglion size, the fraction of the non-wetting fluid in the form of mobile ganglia, the ratio of the conventional relative permeability coefficients and the fractional flows were studied as functions of the system parameters and were correlated with the flow phenomena at pore level and the system factors.

Concluding, by the mid 90s the Payatakes group has succeeded in developing theoretical and semi-analytical models that described and explained the basic phenomena and the flow mechanisms occurring in steady-state two-phase flow in porous media and regulating the transport of the two phases. The results of the experimental studies, especially those of Avraam and Payatakes (1995, 1999), implied that a fundamental reconsideration of fractional flow theory was warranted and that any theoretical model of two-phase flow in porous media should take into account the detailed microscopic flow mechanisms, if it is meant to be true-tonature.

#### The DeProF Evolution Period

A first step towards developing a new true-to-nature model was to try to explain on rigorous physical background the results/observations of the experimental studies of Avraam *et al.* (1994), Avraam and Payatakes (1995, 1999) and especially those pertaining to the mutation of the flow regimes – characterizing the total flow – over the range of the values of the operational variables, *i.e.* to explain the variation of the flow patterns observed as the system is operated in different states. The *DeProF* true-to-mechanism model emerged as a "by-product" of this research effort.

The aforementioned experimental work has shown the existence of three basic flow regimes (patterns) during immiscible steady-state two-phase flow through porous media, namely GD (Ganglion Dynamics), DTF (Drop Traffic Flow) and CPF (Connected-oil Pathway Flow). The key difference between these regimes is the degree of disconnection of the non-wetting phase which, in turn, affects the relative magnitude of the rate of energy dissipation caused by capillary effects compared to bulk viscous stresses. The actual flow is usually a mixture of at least two of the basic flow patterns. Each flow pattern prevails over mesoscopic regions of the porous medium space (ranging from a few to a few hundred pores), whereas the macroscopic flow is perfectly homogeneous. In the DeProF model, each flow pattern is modeled by a prototype flow and the novel concept of the decomposition of the overall flow in prototype flows (the origin of the *DeProF* acronym) was introduced. In the first versions of the DeProF model (Payatakes & Valavanides, 1998 and Valavanides & Payatakes, 2001), the DOF included only Ganglion Dynamics (GD) whereas in a follow-up work (Valavanides & Payatakes, 2000), results were presented for the case where DOF includes the motion of ganglia as well as of droplets. All basic pore scale flow mechanisms are incorporated in the macroscopic flow characterization functions of the prototype flows. The gap between micro- and macroscopic flow characterization is bridged with the application of the Effective Medium Theory (EMT). Then, all physically acceptable (internally constrained) combinations of the flow patterns are readily determined. Postulating that each physically acceptable flow combination has the same probability of being "visited", we can evaluate the mean macroscopic relative contribution of each pattern to the total flow. A direct application of the analysis leads to the *ab initio* theoretical determination of the conventional relative permeability coefficients. This method (DeProF) predicts, quantitatively, the strong dependence of the relative permeabilities (for a given porous medium) not only on the saturation but also on the capillary number, the viscosity ratio, the contact angles, etc. The entire procedure is very fast; the calculation for a given set of parameters requires about 3-4 min with a contemporary personal computer. The basic aspects of the *DeProF* model are presented in the next section.

The predictive capability of the *DeProF* model was used to examine the effect of network dimensionality and wettability (Valavanides & Payatakes, 2002 a,b and 2004) and to investigate whether Optimum Operating Conditions (OOC) appear in steady-state two-phase flow in pore networks (Valavanides and Payatakes, 2003). A new macroscopic dependent variable was defined, namely the energy utilization factor. This variable is defined as the ratio of the reduced o/w flow rate ratio over the reduced mechanical energy dissipated; it represents a measure of the efficacy of the physical process in terms of oil transport. Using DeProF, simulations were carried out over the domain of capillary number, Ca and oil-water flowrate ratio, r, in which twophase flow is sustainable and for three systems of oil/water/ pore network. The results show that, for every system, there exist a continuous line (locus) in the (Ca, r) domain on which the energy utilization factor attains a local maximum.

Then, the next task was to introduce a rational justification of the existence of the locally Optimum Operating Conditions predicted by the *DeProF* theory (Valavanides, 2010). steady-state two-phase flow in porous media is a stationary process maintained in dynamic equilibrium on the expense of energy supplied to the system (an off-equilibrium process). The efficiency of the process depends on its spontaneity, measurable by the rate of global entropy production. The latter is the sum of two components: the rate of mechanical energy dissipation at constant temperature and a component of conformational entropy production, directly related to the number of internal flow arrangements. The *DeProF* algorithm simulations indicated that for every oil-water-pore network system, Optimum Operating Conditions (OOC) exist for the  $r^*(Ca)$  values for which the rate of global entropy production becomes maximum, *i.e.* when the process is as spontaneous as physically possible. The conceptual statement introduced was an initial approach towards implementing aspects of statistical thermodynamics to elucidate further the underlying physics of the sought process.

The mechanistic model *DeProF* predicts the relative permeabilities using the concept of decomposition in prototype flows; it accounts for the pore-scale mechanisms and the network wide cooperative effects and is sufficiently simple and fast for practical purposes. The sources of non-linearity (which are caused by the motion of interfaces) and other complex effects are modeled satisfactorily. The quantitative and qualitative agreement between existing sets of data and the corresponding theoretical predictions of the *DeProF* model is excellent (Valavanides and Payatakes, 2000, 2001).

How much does the *DeProF* model depend on the findings/results/observations of precursor experimental studies and/or modeling efforts? The *DeProF* model is a self-consistent independent true-to-mechanism model; there are no adjustable parameters in *DeProF* (no calibration needed); it inherited only the qualitative aspects of the findings in precursor studies *i.e.* the fact that the macroscopic flow is a mixture of prototype flows, that mobilized ganglia tend to align with the macroscopic flow, that the ganglion size distribution decays with ganglion size and, last but not least, that mobilization of stranded ganglia may be intrigued at Ca values substantially lower than the threshold values expected for solitary ganglion mobilization.

#### 1 THE DeProF THEORY

#### 1.1 Basics of the DeProF Model

In the *DeProF* model it is assumed that, in the most general case, the macroscopic flow can be decomposed into two prototype flows, Connected-oil Pathway Flow (CPF) and Disconnected Oil Flow (DOF). The latter comprises Ganglion Dynamics (GD) and Drop Traffic Flow (DTF), regimes which have been observed experimentally (Avraam and Payatakes, 1995, 1999; Tallakstad *et al.*, 2009). Each prototype flow has the essential characteristics of the corresponding flow patterns in suitably idealized form and so the pore scale mechanisms are incorporated in the prototype flows.

In the general case of SS2 $\varphi$ FPM of Figure 2a, oil and water are continuously supplied along the macroscopic flow direction,  $\tilde{z}$ , with constant flowrates  $\tilde{q}_{a}$  and  $\tilde{q}_{w}$ .

In the CPF region, the oil retains its connectivity and flows with virtually one-phase flow. The porous medium volume fraction occupied by the connected oil is denoted by  $\beta$ .

The DOF regime is defined as the region composed of the rest of the unit cells, so the DOF volume fraction equals  $(1-\beta)$ (*Fig. 2b*). Water is the wetting phase and always retains its connectivity. DOF implicitly represents the Connected-water Pathway Flow. A microscopic scale representation (a snapshot) of a typical DOF region is shown in Figure 2c. An oil ganglion having a typical "cruising" configuration (Valavanides and Payatakes, 2000, 2001) is shown at the center. All the cells that accommodate parts of this (or any other) oil ganglion are called ganglion cells and are demarcated with a thick dashed line. The rest of the cells in the DOF region are cells containing water and oil drops. These cells comprise the regions of the GD and DTF domains respectively.

The fraction of all the ganglion cells over all the DOF region cells is denoted by  $\omega$  and is called the GD domain fraction. The DTF domain fraction in the DOF region equals  $(1-\omega)$ .  $S_w$ ,  $\beta$  and  $\omega$  are called Flow Arrangement Variables (FAV) because these provide a coarse indication of the prevailing flow pattern. One of the objectives of *DeProF* is to determine the values of  $S_w$ ,  $\beta$  and  $\omega$  that conform with the externally imposed conditions (Ca, *r*).

The flow analysis is carried out at two length scales, a macroscopic scale (10<sup>12</sup> pores or more) and a microscopic scale, and produces a system of equations that includes macroscopic water and oil mass balances, flow arrangement relations at the macroscopic scale, equations expressing the consistency between the microscopic and macroscopic scale representations in the DOF region and an equation that is obtained by applying Effective Medium Theory (Kirkpatrick, 1973) to the "equivalent one-phase Flow" in the DOF (GD and DTF) region - implicitly representing the transfer function for this region (Valavanides and Payatakes, 2000, 2001). The system is closed by imposing an appropriate type of distribution function for the ganglion volumes, which is dictated by the physics of Ganglion Dynamics, experimental observations (Avraam and Payatakes, 1995, 1999; Tallakstad et al., 2009), network (Constantinides and Payatakes, 1996) and numerical simulations (Valavanides et al., 1998).

Using the *DeProF* model, one can obtain the solution to the problem of steady-state two-phase flow in porous media in the form of the following transfer function:

$$x = x \left( \operatorname{Ca}, r; \kappa, \theta_A^0, \theta_R^0, \mathbf{x}_{p.m.} \right)$$
(1)

where,  $x = (-\partial \tilde{p}/\partial \tilde{z})\tilde{k}(\tilde{\gamma}_{ow}Ca)^{-1}$  is the reduced macroscopic pressure gradient,  $\tilde{k}$  is the absolute permeability of the porous medium, Ca is the capillary number, defined as  $Ca = \tilde{\mu}_w \tilde{U}_w / \tilde{\gamma}_{ow}$ ( $\tilde{\mu}_w$  is the viscosity of water,  $\tilde{U}_w$  is the superficial velocity of water and  $\tilde{\gamma}_{ow}$  is the interfacial tension),  $r = \tilde{q}_o/\tilde{q}_w$  is the oil/water flowrate ratio,  $\kappa = \tilde{\mu}_o/\tilde{\mu}_w$  is the oil/water flowrate ratio,  $\kappa = \tilde{\mu}_o/\tilde{\mu}_w$  is the oil/water viscosity ratio,  $\theta_A^0$  and  $\theta_R^0$  are the advancing and receding contact angles and  $\mathbf{x_{p.m.}}$  is a parameter vector composed of all the dimensionless geometrical and topological parameters of the porous medium affecting MS Valavanides / Steady-State Two-Phase Flow in Porous Media: Review of Progress in the Development of the DeProF Theory Bridging Pore to Statistical Thermodynamics Scales

the flow (*e.g.* porosity, genus, coordination number, normalized chamber and throat size distributions, chamber-to-throat size correlation factors, etc.). In the definition of the reduced macroscopic pressure gradient, the term  $(\tilde{\gamma}_{ow}Ca)/\tilde{k}$  represents the pressure gradient for one-phase flow of water at superficial velocity  $\tilde{U}_w$ . Note that, in Equation (1),  $S_w$  is not considered to be an independent variable; actually,  $S_w$  is one of the dependent variables in the system of *DeProF* equations. A typical dependence of *x* on Ca and *r* is presented in Figure 3b for a system with o/w viscosity ratio  $\kappa = 1.45$ .

### 1.2 Physically Admissible Flow Configurations and Mean Macroscopic Flow Variables

A core feature of the *DeProF* model is the detection of all flow configurations – each represented by a triple of values of the flow arrangement variables  $\{S_w, \beta, \omega\}$  – that are physically admissible under the imposed macroscopic flow conditions. On a mesoscopic scale (say 10<sup>4</sup>-10<sup>9</sup> pores), the actual flow at a given region of the porous medium "wanders" within the domain of physically admissible flow configurations



Figure 2

a) "Actual" flow; b) its theoretical decomposition into prototype flows: CPF and DOF; c) a microscopic scale representation (snapshot) of a DOF region. An oil ganglion of size class 5 is shown. For simpler representation, all cells are shown identical and the lattice constant is shown expanded. The dashed line separates the GD cells domain and the DTF cells domain. In reality chambers and throats have prescribed size distributions (Valavanides and Payatakes, 2000).



Figure 3

a) Reduced mechanical power dissipation, *W*, b) reduced pressure gradient, *x* of the total flow, as a function of Ca and *r*. The diagrams pertain to 3-D pore network simulations for an o/w system with viscosity ratio  $\kappa = 1.45$  (Valavanides and Payatakes, 2003).

"visiting" any one with equal probability or frequency (ergodicity).

To detect these flow configurations one may partition the domain  $\{S_w, \beta, \omega\}$  of all possible values of the flow arrangement variables using sufficiently fine steps to obtain a 3-D grid. Then, he may select any triple of values for the flow arrangement variables  $\{S_{w}, \beta, \omega\}$  from this grid and solve the system of the DeProF equations to compute the reduced macroscopic pressure gradient, x', corresponding to that triple of flow arrangement variables. Now, if a solution to the *DeProF* equations that is compatible with the selected  $\{S_w, \beta, \omega\}$  values, exists, this is allowed as a Physically Admissible Solution (PAS) and is denoted as  $x'(S_{w}^{\prime},\beta',\omega')$ . Otherwise, the set of  $\{S_w, \beta, \omega\}$  values is rejected as a possible flow arrangement. The process is repeated until all the grid points have been so characterized. In the end, a domain of the  $\{S_w, \beta, \omega\}$  space is formed, denoted  $\Omega_{PAS}$ , that corresponds to the Physically Admissible Solutions. At any one set of imposed values of the operational parameters (Ca, r), the domain of physically admissible solutions,  $\Omega_{PAS}$ , is a canonical ensemble.

The measure ("volume") of  $\Omega_{PAS}$  is given by:

$$V_{\Omega_{\text{PAS}}}\left(\text{Ca},r\right) = \iiint_{\Omega_{\text{PAS}}\left(\text{Ca},r\right)} dS_{w} d\beta d\omega$$
(2)

where  $\Omega_{PAS}(Ca, r)$  stands for integration carried over the physically admissible ranges in  $(S_w, \beta, \omega)$  for the imposed Ca, r values. The volume of  $\Omega_{PAS}$  is a measure of the degrees of freedom of the process; it is also related to the rate of entropy production at the mesoscopic scale (configurational entropy – see also *Sect. 2.1*).

By assuming that each physically admissible solution is visited with the same probability, or frequency (assumption of ergodicity) and averaging over their domain,  $\Omega_{PAS}$ , a unique solution for the macroscopic flow is obtained. For any quantity,  $\Phi$ ', the corresponding expected mean macroscopic flow quantity,  $\Phi$ , is defined as:

$$\Phi(\operatorname{Ca}, r) = \langle \Phi' \rangle = \frac{\iint_{\Omega_{PAS}(\operatorname{Ca}, r)} \Phi'(\operatorname{Ca}, r) dS_{w} d\beta d\omega}{\iint_{\Omega_{PAS}(\operatorname{Ca}, r)} dS_{w} d\beta d\omega}$$

$$= \frac{1}{V_{\Omega_{PAS}}(\operatorname{Ca}, r)} \iint_{\Omega_{PAS}(\operatorname{Ca}, r)} \Phi'(\operatorname{Ca}, r) dS_{w} d\beta d\omega$$
(3)

A prime is used to denote physically admissible values of any quantity. The symbol without a prime is reserved for the expected value of the quantity.

As with any macroscopic physical quantity, unique set of values for  $S_w$ ,  $\beta$ ,  $\omega$  can be obtained by averaging over the PAS domain. These values define the flow configuration of the mean macroscopic flow.

A physical quantity, that is basic in the analysis of process efficiency, is the reduced rate of mechanical energy dissipation, *W*, defined as the ratio of the specific rate of mechanical energy dissipation of the two phase flow,  $\widetilde{W}$  and of the corresponding rate for one-phase flow of water,  $\widetilde{W}^{1\Omega} = (\widetilde{\gamma}_{ow} \text{Ca})^2 / (\widetilde{k} \widetilde{\mu}_w)$  (see *Eq. A.4* in *Appendix*):

$$W \equiv \widetilde{W}\widetilde{k}\widetilde{\mu}_{w}(\widetilde{\gamma}_{ow}Ca)^{-2}$$
(4)

The rate of mechanical energy dissipation equals the mechanical power that is externally supplied to the system. Mechanical energy dissipation is caused interstitially: by bulk viscous stresses in combination with the local rates of deformation and by capillary pressure in combination with the velocities of moving menisci and contact angle hysteresis effects. Clearly, the relative magnitude of the two contributions depends – among other factors – on the degree of disconnection of oil (the non-wetting phase).

The latter is accounted by a set of physical quantities that are important in flow characterization and in describing the extent of irreversible phenomena associated with the motion of o/w interfaces. These are:

- the reduced superficial velocity of o/w interfaces,  $U_{ow}^{DOF}$ ;
- the coefficient of oil fragmentation,  $f_{OF}$ , (defined as the ratio of the actual interfacial area within the Disconnected Oil Flow (DOF) region over the interfacial area that would be produced if all the oil were fragmented in droplets in the *DeProF* model the size of the oil droplets is correlated to the throat diameter of the pore network);
- the fraction of interface transfer through Drop Traffic Flow,  $\xi_{ow}^D$ , which is a measure of the contribution of droplets in the transfer of o/w interface in two-phase Flows – whereas that of the contribution of ganglia equals  $(1-\xi_{ow}^{D})$  (Valavanides and Payatakes, 2000). A similar physical quantity, namely the specific interfacial area (defined as the ratio of fluid-fluid interfacial area to the total volume of the porous media domain), was introduced by Hassanizadeh and Gray (1993) as a state variable in their thermodynamically derived theory for two-phase flow in porous media, suggesting the possibility to define a unique relation between capillary pressure, saturation and interfacial area. Recently, there are studies investigating such a relation by implementing a dynamic pore-network model. (Joekar-Niasar and Hassanizadeh, 2011, 2012). To this end it would be interesting to elaborate on the affinities between the two approaches.

Typical results of *DeProF* model simulations are presented in Figures 3-5. For economy of space results are only presented for simulations pertaining to o/w systems with viscosity ratios  $\kappa = 1.45$  and for 2-D and 3-D pore networks of the chamberand-throat type described in (Valavanides and Payatakes, 2002, 2003). All the simulations (pertaining to all the examined viscosity ratios) show a systemic consistency. The (Ca, *r*) domain for which two-phase flow is not sustainable or physically admissible is also mapped. The *DeProF* model predictions for the reduced macroscopic pressure gradient, *x* and the mechanical power dissipation, *W*, are presented in



Figure 4

a) Reduced superficial velocity of o/w interfaces,  $U_{ow}^{DOF}$ ; b) coefficient of oil fragmentation,  $f_{OF}$ ; c) fraction of interface transfer through Disconnected Oil Flow (DTF),  $\xi_{ow}^{D}$ , as a function of Ca and r. The diagrams pertain to 3-D pore network simulations for an o/w system with viscosity ratio  $\kappa = 1.45$  (Valavanides and Payatakes, 2002).

Figure 3. It is clear that the effects of capillarity and flowrate ratio are significant up to at least 1 order of magnitude. Results for variables describing the motion of o/w interfaces,  $U_{ow}^{DOF}, f_{OF}, \xi_{ow}^{D}$ , are presented in Figure 4.

The *DeProF* predictions were benchmarked against the experimental data of Avraam and Payatakes (1995) in terms of the reduced mechanical dissipation (*Fig. 5*). The agreement between *DeProF* predictions and laboratory measurements is excellent.

The simulations covered a rectangular domain in (Ca, r), from (Ca, log r) = (10<sup>-7</sup>, -1) to (Ca, log r) = (10<sup>-5</sup>, 2). The domain was covered in successive steps of Ca = 10<sup>-6</sup> (10 steps in the Ca range) and of log r = 0.1 (32 steps in the log rrange). Values of the reduced mechanical power dissipation, were tabulated as  $W_{ij}(Ca_i, r_j)$ . These tabulated values can be interpolated by a general expression of the form:

$$W(\operatorname{Ca}, r) = \begin{cases} A(r)(10^{6} \operatorname{Ca})^{-B(r)} & r \le r_{\lim}(\operatorname{Ca}) \\ n/a & r > r_{\lim}(\operatorname{Ca}) \end{cases}$$
(5)

where:

$$A(r) = 10^{\sum_{i=0}^{2} A_i (\log r)^i} = 10^{A_0 + A_1 \log r + A_i (\log r)^2 + A_3 (\log r)^3}$$
  
and  $B(r) = B_0 + B_1 \log r$  (6)

are functions of r and  $A_0$ ,  $A_1$ ,  $A_2$ ,  $A_3$ ,  $B_0$  and  $B_1$  are appropriate interpolation coefficients, that take values according to the system parameters and:

$$\log[r_{\rm lim}({\rm Ca})] = C(\kappa) {\rm Ca}^{D(k)} \quad \Leftrightarrow \quad r_{\rm lim}({\rm Ca}) = 10^{C(\kappa) {\rm Ca}^{D(k)}}$$
(7)

are the limiting values of the flowrate ratio, r, for which twophase Flow is sustainable (or "physically acceptable"). Similar expressions can easily be derived for the reduced macroscopic pressure gradient *x*, the relative permeabilities,  $k_{ro}$  and  $k_{rw}$ , the specific interfacial area, the plurality of the Physically Admissible Solutions (PAS),  $N_{PAS}$ , etc.

For the system with  $\kappa = 1.45$  (corresponding to the diagram of *Fig. 3a*) the values of the interpolation coefficients (*Eq. 11-14*) are presented in Table 1.

TABLE 1

Values of the coefficients interpolating the *DeProF* model predicted reduced mechanical power dissipation W(Ca, r) (*Eq. 11-14*) for a system with  $\kappa = 1.45$ 

		<b>κ</b> = 1.45		
i	$A_i$	$B_i$	С	D
0	1.8347	0.7138	1.7786	-0.3726
1	0.5717	-0.1292	-	-
2	0.3227	-	-	-
3	0.0427	-	-	-

#### 1.3 Optimum Operating Conditions for SS2φF in Pore Networks

The efficiency of the process with respect to the maximization of the oil transport per kW of mechanical power supplied to the system may be assessed by the values of the energy utilization coefficient,  $f_{EU}$ , a macroscopic quantity defined by Valavanides and Payatakes (2003) (see Eq. A.5-A.7 in Appendix) as:

$$f_{\rm EU} = r/W \tag{8}$$





Reduced mechanical power dissipation, *W*, as predicted by the *DeProF* model (thick line) *vs* actual mechanical power dissipation (bold triangles) measured in the experimental work of Avraam and Payatakes (1995). Thinner lines represent the mechanical power dissipation in the three prototype flows CPF, GD and DTF (Valavanides and Payatakes, 2000). Top row diagrams pertain to systems with viscosity ratio  $\kappa = 1.45$  and bottom diagrams to systems with  $\kappa = 3.35$ . Diagrams on the left pertain to capillary number  $Ca = 1.19 \times 10^{-6}$  and diagrams on the right to  $Ca = 4.75 \times 10^{-6}$ . The agreement between *DeProF* predictions ( $\neg \neg$ ) and laboratory measurements ( $\bigtriangledown$ ) is excellent.

Simulations implementing the *DeProF* model, suggest that conditions of optimum operation (read: improved efficiency) exist for processes of steady-state two-phase flow in pore networks. The term "Optimum Operating Conditions" (OOC) is introduced to interpret those values of Ca and r (the operating parameters) for which the process efficiency, expressed in terms of "oil transport per kW of mechanical power supplied to the process" or "oil produced per kW of mechanical power dissipated in pumps" or "oil flowrate per unit energy cost", takes one (or many) locally maximum values.

The effect of Ca and r on the energy utilization factor  $f_{\rm EU}$  (= r/W) is depicted by the hump-shaped surfaces in the diagrams of Figure 6. For every fixed value in Ca, there exists a unique value in r,  $r^*$ (Ca), for which  $f_{\rm EU}$ (= r/W) attains a locally maximum value. Therefore, a continuous







line  $r = r^*$  (Ca;  $\kappa$ ,  $\theta_A^0$ ,  $\theta_R^0$ ,  $\mathbf{x}_{pm}$ ) exists in the (Ca, *r*) domain for which the energy utilization factor takes locally maximum values and the system is at its most efficient operation in terms of oil flowrate per unit energy cost. This line appears when the *r*/*W* surface ridge is projected on the (Ca, *r*) plane.

The existence of "optimum conditions" for oil transport in steady-state two-phase flow in pore networks is a consequence of the remarkable internal adaptability of the flow to externally imposed flow conditions (Ca, r) and its inherent characteristic in trading-off between Connected Pathway Flow (CPF), Ganglion Dynamics (GD) and Drop Traffic Flow (DTF) and self adjusting the connected *versus* disconnected moving-oil balance.

Detecting and setting Optimum Operating Conditions in (OOC) a real process could eventually increase the process efficiency; that, in turn, could provide potentially large

marginal benefits in industrial applications, such as EOR (Taber *et al.*, 1997a, b). It is therefore imperative to challenge the *DeProF* theory claims regarding the existence of Optimum Operating Conditions (OOC) in such processes and furnish a conceptual justification of the existence of such conditions.

# 2 RECENT PROGRESS: CONCEPTUAL JUSTIFICATION OF THE EXISTENCE OF OPTIMUM OPERATING CONDITIONS

The consistency of *DeProF* model predictions pertaining to Optimal Operation Conditions (OOC) was examined against phenomenological arguments by Valavanides and Payatakes (2003), whereas, recently, the consistency of the *DeProF* model predictions was benchmarked against axioms and/or laws of physics that are not incorporated in the *DeProF* theory and against empirical facts (experimental work). Statistical thermodynamics aspects of the process were examined by Valavanides (2010). In addition, an ongoing retrospective examination of the universal relative permeability curves for SS2 $\varphi$ FPM, in light of the *DeProF* theory predictions, reveals that the existence of Optimum Operating Conditions is also an inherent characteristic of steady-state two-phase flows in real porous media (Valavanides, 2011).

# 2.1 Statistical Thermodynamics Aspects of OOC (the *aSaPP* Concept)

Steady-state two-phase flow in porous media is an off equilibrium process. One needs to provide energy to the process to keep it stationary at fixed operating conditions, *i.e.* to maintain its operation at fixed values of Ca and r (and at fixed temperature, say  $T_0$ ).

A justification of the existence of Optimum Operating Conditions (OOC) was proposed by Valavanides (2010) along the lines of the following postulate (Atkins, 1984):

Spontaneity, the notional inverse for irreversibility, may be quantitatively assessed by the amount of entropy produced globally. Therefore, what the Postulate (P) implies is that, in order to maximize the efficiency of a process under specified operational constraints, one should maximize the process spontaneity or, in other words, minimize its irreversibility.

According to the inductive reasoning presented by Valavanides (2010), the energy utilization coefficient,  $f_{EU} = r/W$  and the global entropy production,  $S_{UNIV}$ , (process spontaneity) show similar dependencies on the operational parameters Ca and *r*, *i.e.*:

$$S_{\text{UNIV}}(\text{Ca},r) \propto f_{\text{EU}}(\text{Ca},r)$$
 (9)

and the latter analogy may be rewritten in terms of quantities that can be evaluated by means of the *DeProF* algorithm (see *Eq. A.9-A.11* in *Appendix*) as:

$$\frac{W(\operatorname{Ca},r)}{T} + k_{DeProF} \ln \left[ N_{\operatorname{PAS}} \left( \operatorname{Ca},r \right) \right] \propto f_{\operatorname{EU}} \left( \operatorname{Ca},r \right) \quad (10)$$

where  $k_{DeProF}$  is a constant quantity – similar in nature to Boltzmann's constant in the statistical thermodynamics definition of entropy – yet to be derived in accordance with the *DeProF* theory on SS2 $\varphi$ FPM, and  $N_{PAS}$  is the actual number of different mesoscopic flow arrangements consistent with the macroscopic flow at (Ca, *r*).

In order to maximize the efficiency of the process one should increase/maximize the sum on the left side of Equation (10). Of the sum components, the first term represents the cost of energy irreversibly transformed into heat and released to the surroundings; any increase of this term should be avoided – even better, this term should be decreased as much as possible. To do so and in parallel, increase as much as possible the total entropy in the universe, in order to increase the efficiency of the process, one may arrange or even "force" the process to operate in such conditions for which the flow is *optimally rich* in different physically admissible mesoscopic flow arrangements. This latter sentence delineates the *aSaPP* ("as Spontaneous as Physically Possible") concept.

#### 2.2 Latent Experimental Evidence of the Existence of Optimum Operating Conditions

A retrospective examination of the universal relative permeability curves for SS2 $\varphi$ FPM, in light of the *DeProF* theory predictions, reveals that the existence of Optimum Operating Conditions (OOC) is actually an inherent characteristic of steady-state two-phase flows in real porous media (Valavanides, 2011). To advocate the previous statement relative permeability diagrams for SS2 $\varphi$ FPM published in the literature had to be examined. For each set of  $\{k_{ro}(S_w), k_{rw}(S_w)\}$  values, a straightforward analysis (see *Eq. A.3, A.8 Appendix*) determines the corresponding values of the flowrate ratio, *r* and the energy utilization coefficient,  $f_{EU} = r/W$ , to be:

$$r = \frac{1}{\kappa} \frac{k_{ro}}{k_{rw}}, \quad f_{\rm EU} = \frac{r}{W} = k_{ro} \left( \frac{k_{ro}}{k_{rw}} + \kappa \right)^{-1}$$
(11)

Every set { $f_{EU}$ , log r} corresponding to { $k_{ro}(S_w)$ ,  $k_{rw}(S_w)$ } through Equation (11), presents a local maximum; this local maximum corresponds to the cross-over point in the relative permeabilities diagram. To date, 23 relperm diagrams in total, from 7 published experimental works referencing different types of pore networks and real porous media, have been examined (results are not presented here due to space limitations but are readily available upon request).



Figure 7

a) Relative permeability vs water saturation measurements for Steady-State two-phase co-current Flow in a fine sand pack, represented by the upper swarm of points (filled rectangles and circles) as published by Bentsen (2005); b) The respective values of the energy utilization coefficient,  $f_{EU}$ , and the flowrate ratio, r, as computed by Equation (11). It is obvious that there exist a locally Optimum Operation Condition, corresponding to the cross-point of the relperm diagrams. The viscosity ratio is  $\kappa = 0.075$  (Valavanides, 2011).

In all cases examined, each set of relperm diagrams transforms through relations (11) into a corresponding diagram,  $f_{\rm EU}(r)$ , similar to that exhibited in Figure 7b and shows the existence of a local maximum. Moreover, diagrams similar to that in Figure 7b, in general correspond to a lateral curved "slice" cut-out of an  $f_{\rm EU}({\rm Ca}, r)$  diagram, similar to that presented in Figure 6. This is so because most of the relative permeability curves published in the literature are furnishing permability measurements at steady-state conditions but at different values of the capillary number.

Tracing and reviewing published experimental work on steady-state two-phase flow in model pore networks, sand packs, real porous media, etc., including any relative permeability diagrams, is an on going project with the objective to benchmark the validity and eventually to verify – in the broadest extent possible – the *DeProF* predictions relative to the existence of Optimum Operating Conditions and to reveal any associated trends with respect to the operational and system parameters. To this end, disclosure or reference of any relative permeability measurements is really welcome by the author.

#### CONCLUSIONS

The *DeProF* theory, developed in the recent past, culminates the Payatakes group research efforts on elucidating the physics of two-phase flow in porous media. It implements mechanistic modeling to bridge the microscale flow mechanisms to macroscale phenomenology in a consistent manner; it is backboned by rigorous theoretical analysis, deductive reasoning and experimental evidence.

Within the context of the proposed *DeProF* theory for steady-state two-phase flow in porous media the following results have been delivered for the first time:

- determination of the system and operational parameters (independent variables) for the sought process (water saturation is not an independent variable, contrary to the conventional knowledge and practice);
- semi-analytical solution of the steady-state two-phase flow in porous media incorporating the determination of the ensemble of physically admissible internal flow arrangements;
- scaling laws (in analytical form) for the macroscopic pressure gradient and the relative permeabilities as a function of the values of system and operational parameters;
- existence and experimental verification of latent Optimum Operating Conditions;
- introduction of a conceptual justification of the existence of Optimum Operating Conditions.
  - The two-phase Flow in Porous Media is "burdened":
- with oil disconnection and capillarity effects that restrain or inhibit – to a certain extent – the superficial transport of oil and water;
- the bulk phase viscosities of oil and water.

Process engineers can take advantage of the natural intrinsic characteristics of two-phase flow in porous media, namely the multitude of internal flows that act as – potentially beneficial – degrees of freedom against the imposed macroscopic constraints. Process engineers must always judge where to set the balance between capillarity or viscosity. Metaphorically speaking, the process designer may trade with the "Daemon" (also know as Nature) – avid for chaos in any form, an amount of configurational chaos (created from the multitude of intrinsic flow arrangements) in exchange for microscopic chaos (dissipating mechanical energy into heat). The *aSaPP* ("as Spontaneous as Physically Possible") concept in essence corroborates the delivery of technical guidelines that may prove especially useful in designing more efficient steady-state two-phase flow processes.

The *DeProF* theory for steady-state two-phase flow in porous media explains unexpected (existence of optimum operating conditions) and unexplained (mutation of prototype flow regimes) observations, raises new problems (of reconciliation, of how to conduct new previously unthought of observational tests), concentrates upon the essentials of the process but without ignoring too many of the real process' qualifying side issues. It therefore has the potential to serve as the current (for-the-time-being) theory for Steady-State two-phase flow in porous media.

An open problem that still needs to be addressed is of "technical" – or computational – nature: specifically the delivery of an expression for the constant  $k_{DeProF}$  appearing in expression (10). To this end, the work of Campisi and Kobe (2010) (in which the Boltzmann principle,  $S_B = k_B \ln \Phi$ , is derived in a contemporary, self-contained and accessible form, based on classical mechanical models of thermo-dynamics) may be implemented. To the author's confidence, delivery of an appropriate expression for  $k_{DeProF}$ , would finally nail-down a robust theory for steady-state two-phase flow in porous media.

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#### APPENDIX

#### Derivation of Relations (4) and (11)

The definition of oil-water flowrate ratio,  $r = \tilde{q}_o/\tilde{q}_w = \tilde{U}_o/\tilde{U}_w$ , when combined with the Darcy fractional flow equations:

$$\tilde{U}^{o} = \frac{\tilde{q}^{o}}{\tilde{A}} = \frac{\tilde{k}}{\tilde{\mu}_{o}} k_{ro} \frac{\partial \tilde{p}}{\partial \tilde{z}} \qquad \tilde{U}^{w} = \frac{\tilde{q}^{w}}{\tilde{A}} = \frac{\tilde{k}}{\tilde{\mu}_{w}} k_{rw} \frac{\partial \tilde{p}}{\partial \tilde{z}}$$
(A.1)

and the experimentally verified condition that in steady-state two-phase fully-developed flow conditions the pressure gradient is the same for both fluids (see Eq. 10, 11) and Figure 1 in Avraam and Payatakes (1999):

$$\frac{\Delta \tilde{p}}{\Delta \tilde{z}}\Big|_{o} = \frac{\Delta \tilde{p}}{\Delta \tilde{z}}\Big|_{w} = \frac{\Delta \tilde{p}}{\Delta \tilde{z}}$$
(A.2)

yields the first of the set of Relations (11):

$$r = \frac{\tilde{q}_o}{\tilde{q}_w} = \frac{\tilde{U}_o}{\tilde{U}_w} = \frac{k_{ro}/\tilde{\mu}_o}{k_{rw}/\tilde{\mu}_w} = \frac{1}{\kappa} \frac{k_{ro}}{k_{rw}}$$
(A.3)

Let  $\widetilde{W}^{1\Phi}$  be the specific mechanical power dissipation (specific as per unit porous medium volume – p.u.v.p.m.) for one-phase Flow of water at an equivalent flowrate,  $\widetilde{q}_w$ , against a porous medium cross section of surface,  $\widetilde{A}$  and along a distance,  $\Delta \widetilde{z}$ , given by:

$$\tilde{W}^{1\Phi} = \frac{\tilde{q}_{w}\Delta\tilde{p}}{\tilde{A}\Delta\tilde{z}} = \frac{\tilde{q}_{w}}{\tilde{A}}\frac{\Delta\tilde{p}}{\Delta\tilde{z}} = \tilde{U}_{w}\frac{\tilde{\mu}_{w}}{\tilde{k}}\tilde{U}_{w} = \frac{\tilde{\mu}_{w}}{\tilde{k}}\left(\frac{\tilde{\mu}_{w}\tilde{U}_{w}}{\tilde{\gamma}_{ow}}\frac{\tilde{\gamma}_{ow}}{\tilde{\mu}_{w}}\right)^{2} = \frac{\left(\mathrm{Ca}\tilde{\gamma}_{ow}\right)^{2}}{\tilde{\mu}_{w}\tilde{k}} \tag{A.4}$$

The specific (p.u.v.p.m.) mechanical power dissipation for the steady-state concurrent two-phase flow of oil and water, at flowrates  $\tilde{q}_o$  and  $\tilde{q}_w$  and with superficial velocities,  $\tilde{U}_o$  and  $\tilde{U}_w$ , within a porous medium cross section of surface,  $\tilde{A}$  and along a distance,  $\Delta \tilde{z}$ , is given by:

$$\begin{split} \tilde{W} &= \frac{\tilde{q}_{o}\Delta\tilde{p}_{o} + \tilde{q}_{w}\Delta\tilde{p}_{w}}{\tilde{A}\Delta\tilde{z}} = \frac{\tilde{q}_{o}}{\tilde{A}}\frac{\Delta\tilde{p}}{\Delta\tilde{z}} \bigg|_{o} + \frac{\tilde{q}_{w}}{\tilde{A}}\frac{\Delta\tilde{p}}{\Delta\tilde{z}}\bigg|_{w} = \tilde{U}_{o}\frac{\tilde{\mu}_{o}}{\tilde{k}k_{ro}}\tilde{U}_{o} + \tilde{U}_{w}\frac{\tilde{\mu}_{w}}{\tilde{k}}\tilde{k}_{rw}\tilde{U}_{w} \\ &= \tilde{U}_{w}^{2}\frac{\tilde{\mu}_{w}}{\tilde{k}}\bigg(r^{2}\frac{\kappa}{k_{ro}} + \frac{1}{k_{rw}}\bigg) = \frac{\left(Ca\tilde{\gamma}_{ow}\right)^{2}}{\tilde{\mu}_{w}\tilde{k}}\frac{1}{k_{ro}}\bigg(r^{2}\kappa + \frac{k_{ro}}{k_{rw}}\bigg) \\ &= \frac{\left(Ca\tilde{\gamma}_{ow}\right)^{2}}{\tilde{\mu}_{w}\tilde{k}}\kappa r\frac{1}{k_{ro}}(r+1) = \frac{\left(Ca\tilde{\gamma}_{ow}\right)^{2}}{\tilde{\mu}_{w}\tilde{k}}\frac{1}{k_{rw}}(r+1) \end{split}$$
(A.5)

Therefore, the reduced mechanical power dissipation for the steady-state two-phase flow of oil and water, W, may be expressed – elegantly – in any of the three equivalent forms:

$$W = \frac{\tilde{W}}{\tilde{W}^{1\Phi}} = \frac{1}{k_{ro}} \left( r^2 \kappa + \frac{k_{ro}}{k_{rw}} \right) = \kappa r \frac{1}{k_{ro}} \left( r + 1 \right) = \frac{1}{k_{rw}} \left( r + 1 \right)$$
(A.6)

The process efficiency, may be defined as the ratio of the recovered oil flowrate,  $\tilde{q}_o = \tilde{U}_o \tilde{A}$ , over the mechanical power dissipation,  $\tilde{W}$ , within a porous medium control volume,  $\Delta \tilde{V} = \tilde{A} \Delta \tilde{z}$ , expressed as  $\tilde{U}_o \tilde{A} (\tilde{W} \tilde{A} \Delta \tilde{z})^{-1}$ . This may be reduced by the respective efficiency for one-phase flow conditions,  $\tilde{U}_w \tilde{A} (\tilde{W}^{1\Phi} \tilde{A} \Delta \tilde{z})^{-1}$ , to define the energy utilization factor,  $f_{\rm EU}$ , a dimensionless macroscopic variable defined as the ratio of the reduced o/w flow rate ratio over the reduced rate of mechanical energy dissipation.

The energy utilization factor is a measure of the process efficiency in terms of oil flowrate per unit energy cost:

$$f_{\rm EU} = \frac{\tilde{U}_o \tilde{A} \left( \tilde{W} \tilde{A} \Delta \tilde{z} \right)^{-1}}{\tilde{U}_w \tilde{A} \left( \tilde{W}^{1\Phi} \tilde{A} \Delta \tilde{z} \right)^{-1}} = \frac{r}{W}$$
(A.7)

and may be expressed in any of the three equivalent forms:

$$f_{\rm EU} = \frac{r}{W} = \frac{k_r^o}{\kappa(r+1)} = k_r^w \frac{r}{r+1} = k_r^o \left(\frac{k_{ro}}{k_{rw}} + \kappa\right)^{-1}$$
(A.8)

#### Derivation of Equation (10)

To proceed with the derivation of Equation (10), we need first to define the physical domains in which the process of steadystate two-phase flow in porous media takes place. We define as:

*System:* the porous medium and the two fluids;

- *Process*: steady-state two-phase flow in the porous medium maintained at stationary (dynamic) equilibrium under fixed Ca and *r*;
- Surroundings: the heat reservoir in which the system resides and with which it exchanges heat at constant temperature, say  $T_0$ . The heat reservoir can absorb all the heat released by the system;

*Universe*: it comprises the system and the surroundings.

The analogy in (9) relates two physical quantities. Of these,  $f_{EU}$  has been already derived from classical mechanics (mass and momentum balances) and computed numerically through Equation (8) by use of the *DeProF* model algorithm, whereas  $S_{UNIV}$  needs first to be derived analytically and then numerically.

The entropy produced globally (within the universe),  $S_{\text{UNIV}}$ , is the sum of two terms: a term representing the entropy released from the system to the surroundings,  $S_{\text{SUR}}$ , and a term representing the entropy produced within the system,  $S_{\text{SYS}}$ . The former is actually produced in the surroundings from the Process occurring within the system (see below); the latter may be directly related to the respective production of chaos due to the multitude of the mesoscopic flow configurations (the PAS of *DeProF* theory) that are maintained for so long as the (stationary) process is kept at conditions of dynamic equilibrium. Therefore:

$$S_{\text{UNIV}}\left(\text{Ca},r\right) = S_{\text{SUR}}\left(\text{Ca},r\right) + S_{\text{SYS}}\left(\text{Ca},r\right)$$
(A.9)

One may proceed by interpreting each source of entropy production as follows. The rate of entropy production in the surroundings (maintained at constant temperature  $T_0$ ),  $S_{SUR}$ , is due to the rate with which mechanical energy is dissipated within the system, W, irreversibly transformed into heat, Q, and then released to the surroundings. Therefore:

$$S_{\text{SUR}}\left(\text{Ca},r\right) = \frac{Q\left(\text{Ca},r\right)}{T_0} = \frac{W\left(\text{Ca},r\right)}{T_0}$$
(A.10)

The second source of entropy,  $S_{\text{UNIV}}$ , is due to the multitude of the mesoscopic flow arrangements maintained within the system process (configurational entropy). It can be expressed similar to the Boltzmann entropy formulation in statistical mechanics:

$$S_{\text{SYS}}\left(\text{Ca},r\right) = k_{DeProF} \ln\left[N_{\text{PAS}}\left(\text{Ca},r\right)\right]$$
(A.11)