



Optimum Operating Conditions for Two-Phase Flows in Pore Networks: Conceptual /Numerical Justification Based on the MEP principle (43)

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Abstract

The mechanistic model *DeProF* considers steady-state two-phase flow in porous media as a composition of three flow patterns: connected-oil pathway flow, ganglion dynamics and drop traffic flow. The key difference is the degree of disconnection of the non-wetting phase which affects the relative magnitude of the rate of energy dissipation caused by capillary effects, compared to that caused by viscous stresses. An appropriate mesoscopic scale analysis leads to the determination of all the internal flow arrangements of the basic flow patterns that are compatible to the externally imposed flow conditions. The observed macroscopic flow is an average over the canonical ensemble of the flow arrangements.

Extensive *DeProF* simulations revealed that there exist a continuous line [a locus, $r^*(Ca)$] in the domain of the process operational variables -the capillary number, Ca , and the oil-water flowrate ratio, r - on which the efficiency of the process (oil produced per kW dissipated in pumps) attains local maxima. Such maxima have been experimentally identified.

Subsequently, the existence of the locally *optimum operating conditions* could be rationally justified by the following *conceptual inference*. Steady state two-phase flow in porous media is an off-equilibrium process. The rate of global entropy production (a measure of the process spontaneity) is the sum of two components: the rate of mechanical energy dissipation at constant temperature (thermal entropy), Q/T , and a Boltzmann-type statistical-entropy production component, $kDeProF \ln \Phi$, directly related to the number of different physically admissible internal flow arrangements, Φ , associated with every flow condition (configurational entropy). By applying the MEP principle we may *infer* that optimum operation of the process is met on a locus of conditions whereby the process total entropy production rate takes maximum values.

To reduce the falsifiability of that inference, one needs to provide numerical evidence. To do so, it is necessary to deliver: (a) an efficient analytical/numerical scheme, to evaluate the number Φ of the different flow arrangements; (b) an expression for the constant $kDeProF$ in the Boltzmann-entropy expression.

Combinatorial considerations provided the analytical background to evaluate the number of different micro-arrangements of the flow per physically admissible solution. The limiting procedure based on Stirling's approximation has been applied to downscale the excessively large computational effort associated with the numerical handling of operations between large factorial numbers. Still, an appropriate application of the Boltzmann principle needs to be implemented, to deliver an expression for the constant $kDeProF$ pertaining to the sought process.



Scope

Immiscible, **two-phase flow in porous media** is the core process in many industrial applications (recovery of hydrocarbons, soil remediation, protection of aquifers, etc.)

A variety of phenomena take place across scales from below the pore scale to the fracture or field scale (*hierarchical system*).

An inherent characteristic of ss2 ϕ fpm is the existence of *optimum operating conditions (OOC)* in terms of *efficiency*.

Scope is to provide a theoretical justification -of the existence of OOC- based on statistical thermodynamics, i.e. the *maximum entropy production (MEP)* principle



Outline

The examined process

Phenomenology & essentials

The DeProF model essentials (in brief)

True-to-mechanism modeling essentials

Predictions of the DeProF model for SS 2 ϕ -f-pm

dp/dz, Rel-Perm, intrinsic flow arrangement /variables

Current issues, Open Problems, Ideas & Challenges in 2 Φ fpm

Retrospective examination of rel-perm. diagrams

Universal Operational Efficiency Map for SS2 ϕ fpm Processes

Normative Characterization of 2 ϕ flows in pm

Justification of phenomenology based on Statistical Thermodynamics Principles

Implementation of different rheology (compressible flows, emulsions, USS, other)

Technical Applications (reconsideration of API/RP40 standard, field geometries etc.)



References

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2. Valavanides & Payatakes, *AWR*, **24**, 385-407 (2001)
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4. Valavanides & Payatakes, *SPE78516* (2002)
5. Valavanides & Payatakes, SCA2003-18 (2003)
6. Valavanides & Payatakes, SPE88713 (2004)
7. Valavanides, SPE135429 ATCE2010 (2010)

The ImproDeProF Project → <http://users.teiath.gr/marval/ArchIII/ImproDeProF.html>

8. **Valavanides, *Oil & Gas Science Technology* 67(5) 2012** ← Review & state-of-the-art
9. Valavanides, SCA2014-047
10. Tsakiroglou *et al.*, SCA2014-041
11. Valavanides *et al.*, RFP 2014, Sept. 2014, Amsterdam, NL.



The examined process: Immiscible, stationary (a.k.a. “steady-state”) two-phase flow in porous media (or networks)

Applications

Oil & H/C industry (upstream/downstream),
soil remediation processes,
Reactors, PEM fuel cells etc.

Phenomenology & essentials

tbd

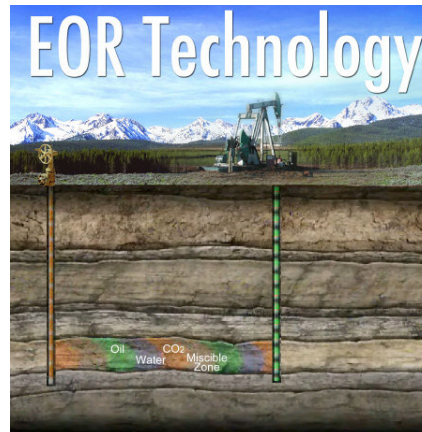
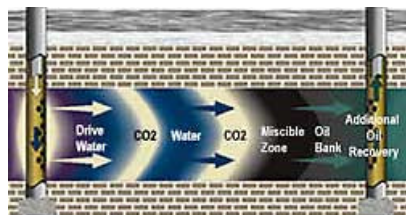


Applications of 2 ϕ FPM

Enhanced Oil Recovery (EOR)

Secondary & Tertiary oil displacement in reservoirs to recover trapped oil (~50% of original oil in place)

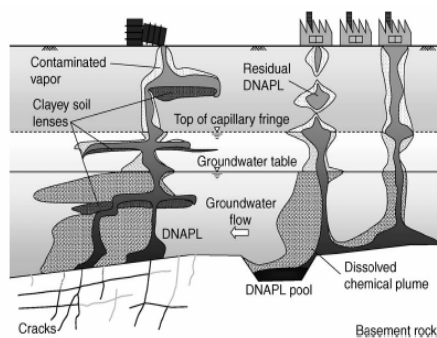
Use of displacing media: CO₂, water + liquid polymers (and combinations), nitrogen, foams, in-place combustion gas etc.



Applications of 2 ϕ FPM

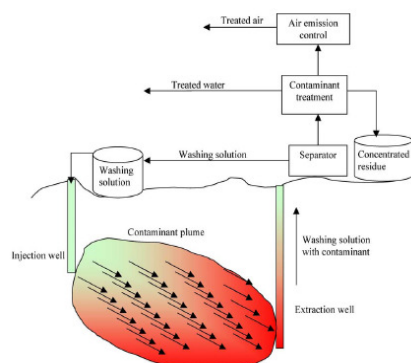
Soil remediation

Problem



Typical DNAPL migration processes
[from Kamon *et al* Engineering Geology **70** (2003)]

Remedy

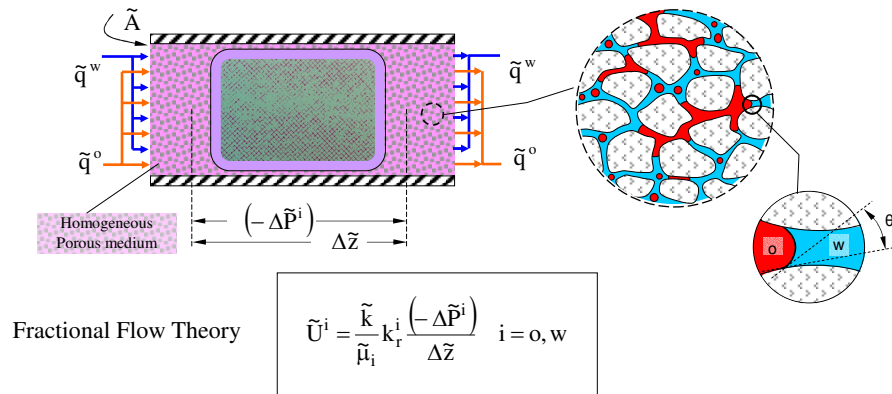


In-situ soil flushing process
[from Khan *et al* J Env Management **71** (2004)]



Statement of the SS2φFPM Problem

Stationary Two-phase Flow in Porous Media



In Conventional Fractional Flow Theory $\rightarrow k_r^i = k_r^i(S_i, \mathbf{x}_{pm})$

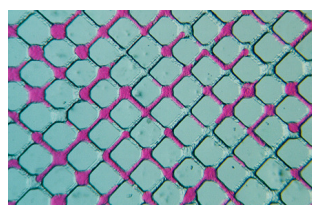
But in reality $\rightarrow$

$$k_r^i = k_r^i(Ca, r; \kappa, \theta_A^0, \theta_R^0, \mathbf{x}_{pm})$$

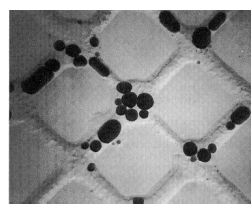


Flow Regimes during Steady-State Two-Phase Flow in Porous Media. Experimental Study (1).

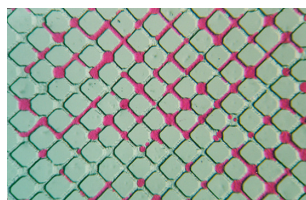
(Avraam & Payatakes, *JFM*, **293**, 207-236, 1995)



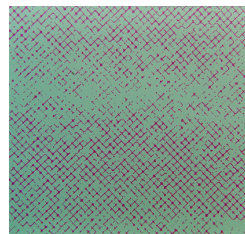
Large Ganglion Dynamics (LGD)



Drop Traffic Flow (DTF)



Small Ganglion Dynamics (SGD)



Connected Pathway Flow (CPF)

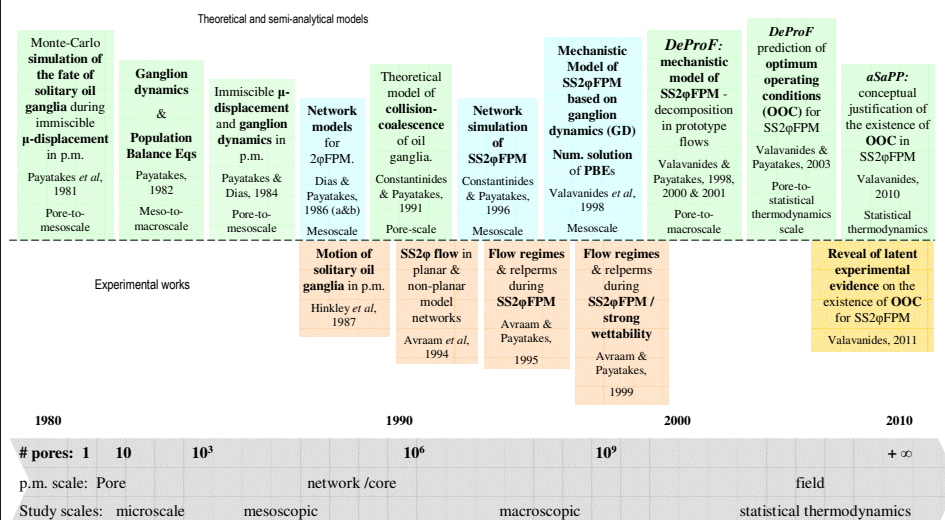


The *DeProF* model essentials



Evolution of *DeProF* theory for steady-state 2phase flow in porous media (SS2 ϕ FPM)

Time- & scale-wise evolution of research leading to the development of the *DeProF* theory





DeProF

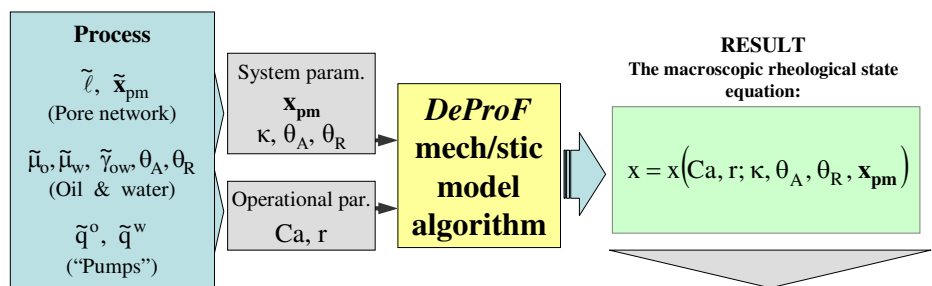
A True-to-mechanism Theoretical Model For Stationary Two-Phase Flow in Porous Media (SS2φFPM)

Modeling essentials

- **D**ecomposition into 3 **P**rototype **F**lows:
Connected-oil **P**athway **F**low & **D**isconnected **O**il **F**low=
(**G**anglion **D**ynamics + **D**rop **T**raffic **F**low)
- Physicochemical characteristics of oil/water/p.m.
- Dynamic wettability (contact angles)
- Mobilization and stranding probabilities for disconnected oil
- Accounting of unit cell Conductivities for all flow configurations
- Implementation of Effective medium theory
- Hierarchical modeling / Scale-up pore-to-”core”-to-field scales
- Physically admissible solutions & ergodicity principles



The “DeProF” model



Reduced Macroscopic
Pressure Gradient

$$x = \frac{\partial \tilde{P}}{\partial \tilde{z}} \frac{\tilde{k}}{\tilde{\gamma}_{ow} Ca}$$

And k_{ro} , k_{rw}
Relative Permeabilities!

Interstitial physical characteristics of SS 2φ flow in pm

S^w , β , ω , **Flow arrangement variables (FAV)**

$\eta^{a,CPF}$, $\eta^{a,G}$ Oil flow rates in CPF & DOF (GD)

$U^{ow,DOF}$ Flowrate of o/w interfaces

f_{OF} Coefficient of oil fragmentation,

$\xi^{ow,D}$ Flowrate of o/w interface through DTF

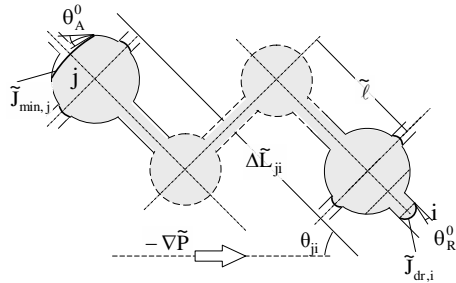
n^G Ganglion size distribution

f_{EU} **Energy utilization factor**



DOF modelling - microscopic scale (2)

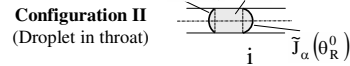
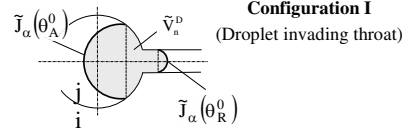
Criterion of Mobilization of Ganglia & Droplets



Ganglion mobilization condition:

$$\tilde{L}_n^G \int_{-\infty}^{+\infty} \left| \frac{\partial \tilde{p}}{\partial \tilde{z}} \right| P(y) dy \geq 2\tilde{\gamma}_{ow} [\tilde{J}_{dr,i}(\theta_R^0) - \tilde{J}_{min,j}(\theta_A^0)]$$

$$\forall j, i = 1, \dots, 5$$



Droplet mobilization condition:

$$\tilde{\ell} \frac{\sqrt{2}}{2} \int_{-\infty}^{+\infty} \left| \frac{\partial \tilde{p}}{\partial \tilde{z}} \right| P(y) dy \geq 2\tilde{\gamma}_{ow} [\tilde{J}_\alpha(\theta_R^0) - \tilde{J}_\alpha(\theta_A^0)]$$

$$\forall \alpha \in \{I, II\}$$

Ganglia & droplets, as members of a dense population, can move even at $Ca \ll 10^{-5}$



DeProF equations

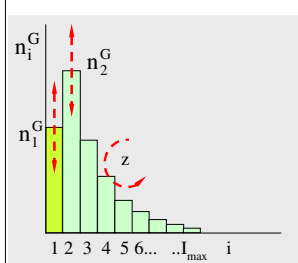
8 equations for ($I_{max}+6$) unknowns

Macroscopic scale	$U^{o,CPF} = \frac{1}{\kappa r} x$	{ Darcy's law in CPF }	(1)
	$(1-\beta)U^{w,DOF} = 1$	{ Total water mass balance }	(2)
	$\beta U^{o,CPF} + (1-\beta)U^{o,DOF} = 1$	{ Total oil mass balance }	(3)
	$\beta + (1-\beta)[\omega S^{o,G} + (1-\omega)S^{o,D}] = 1 - S^w$	{ Total oil (or water) mass arrangement t condition }	(4)
Macro-micro scale consistency	$\sum_{i=1}^{I_{max}} n_i^G N_i^G = 2N_d$	{ Oil ganglion volume normalization condition }	(5)
	$\frac{1}{2} \sum_{i=1}^{I_{max}} n_i^G V_i^G = S^{o,G}$	{ GD oil saturation in terms of ganglion volume distribution }	(6)
	$\sum_{i=1}^{I_{max}} m_i^G m_i^G u_i^G = 2rU^{o,DOF}$	{ Oil ganglion mass balance in DOF }	(7)
Effective Medium Theory in DOF	$\omega \sum_{a,b,i} P_{a,i}^b(x) \frac{k\kappa(1+r) - k\beta x - \kappa(1-\beta)xg_{a,i}^b(x)}{k[\kappa(1+r) - \beta x] + \kappa(1-\beta)xg_{a,i}^b(x)} + (1-\omega) \sum_{a,b} P_a^b(x) \frac{k\kappa(1+r) - k\beta x - \kappa(1-\beta)xg_a^b(x)}{k[\kappa(1+r) - \beta x] + \kappa(1-\beta)xg_a^b(x)} = 0$		{ EMT equation for "Equivalent Water" Flow in DOF } (8)



Closure Scheme

A sharply decreasing ganglion size distribution is *imposed* based on experimental arguments^[1] & theoretical observations^[2,3].



$$n_i^G = \begin{cases} n_2^G z^{(i-2)}, & 3 \leq i \leq I_{\max} \\ 0, & i > I_{\max} \end{cases}$$

n_1^G : variable $\in (0,1)$

n_2^G : variable $\in (0,1)$

$I_{\max}$: such that $\Pr(\text{mobilization } |i \geq I_{\max}|) = 1$

z : exponent that scans all *admissible* values in $(0,1)$

DeProF: 8 equations & 8 unknowns

x

$$\mathbf{U} = \{U^{o,CPF}, U^{o,DOF}, U^{w,DOF}\}$$

$$\mathbf{S} = \{S^{o,G}, S^{o,D}\}$$

$$\mathbf{n}^G = \{n_1^G, n_2^G\}$$



$$x = x(\text{Ca}, r; \kappa, \theta_A^0, \theta_R^0, \mathbf{x}_{pm})$$

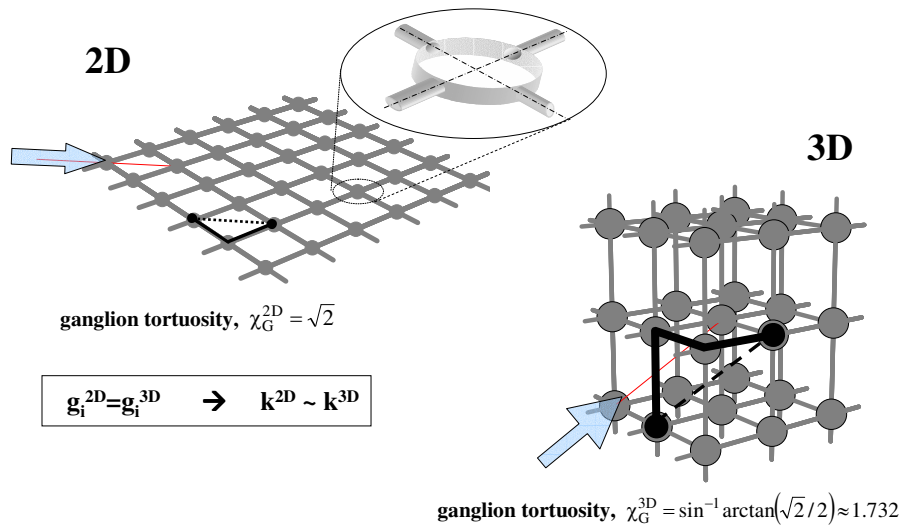
SSFD 2φFPM



**The *DeProF* model predictions
following simulations
for 2ph flow in pore networks**



The pore networks used in simulations



The Domain of Physically Admissible Solutions (PAS) (in DeProF theory)

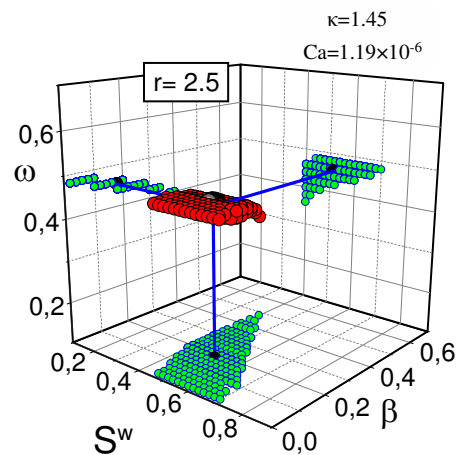
For each set (Ca, r) of system parameter values the 2ϕ flow visits a continuum of physically admissible flow configurations represented by (S^w, β, ω) –the PAS domain (cloud of red balls).

The PAS domain is a *canonical ensemble*

A unique set of values for S^w , β and ω (black balls) are obtained by averaging over the PAS domain.

The **volume of the PAS domain** (red cloud) is a measure

- of the **process number of degrees of freedom** and
- of the **process contribution to configurational entropy**.



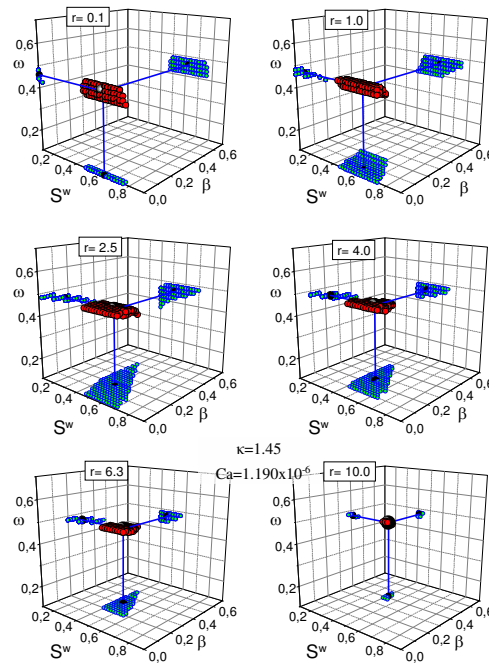


Effect of $r=q^o/q^w$ on the PAS domain (degrees of freedom)

For any fixed value of Ca and as r gradually increases, the PAS domain progressively swells, extends to a max. size and shrinks to zero (just as 2-ph flow cease to be sustainable).

When the PAS domain attains a max. volume, the 2 ϕ flow is as rich as possible in different flow configurations.

A systematic behavior is observed for the other o/w systems examined ($\kappa=0,66$ & $3,35$)

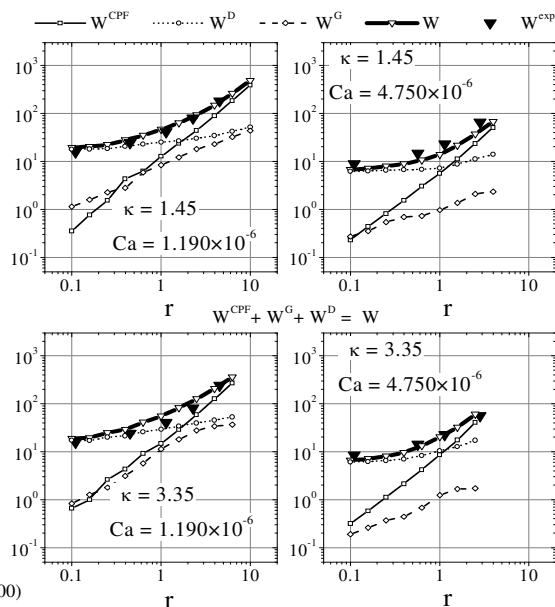


Benchmark: *DeProF* model (—) vs experiment (▼)

Reduced Mechanical Power Dissipation, W

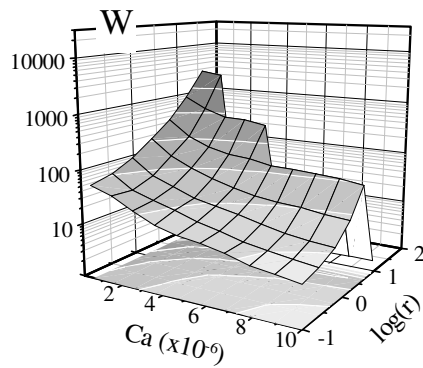
Effect of $Ca=\mu_w U_w/\gamma_{ow}$
& $\kappa=\mu_o/\mu_w$

No adjustable parameters
No interpolation



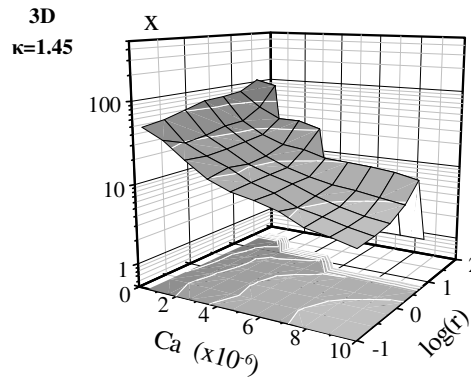


Reduced mechanical power
dissipation of the total flow



$$W = \frac{\tilde{W}}{\tilde{W}^{1\Phi}} = \frac{\tilde{W}\tilde{k}\tilde{\mu}_w}{(\tilde{\gamma}_{ow}Ca)^2}$$

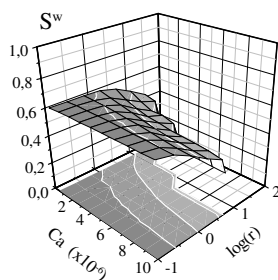
Reduced pressure gradient



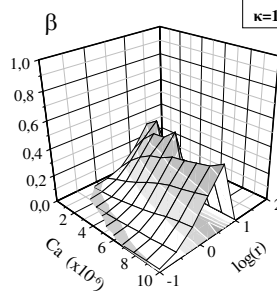
$$X = \frac{\partial \tilde{p}}{\partial \tilde{z}} \frac{\tilde{k}}{\tilde{\gamma}_{ow}Ca}$$



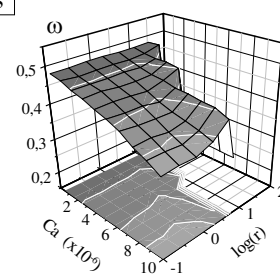
Flow arrangement variables (FAV)



Oil saturation, S^w



Connected-oil
saturation, β
(pm volume fraction
occupied by the
connected oil)



“ganglia saturation”
of the DOF cells, ω
(ganglion cells over all the
DOF region cells)



Macroscopic interstitial flow variables

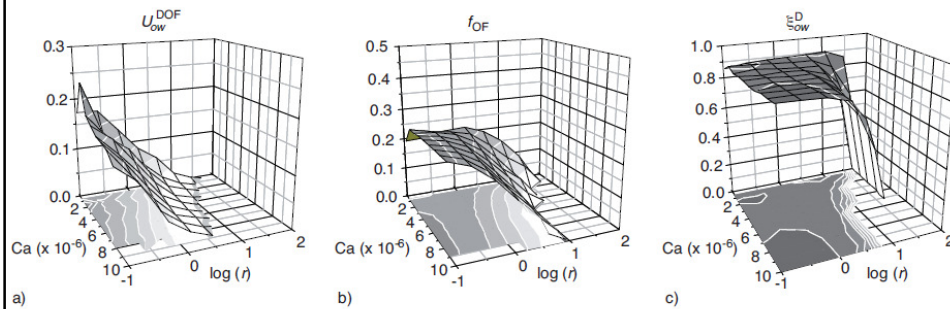


Figure 4

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), ε_D^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).

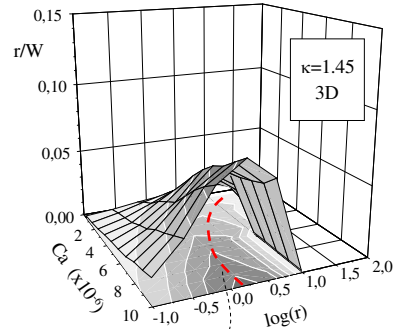
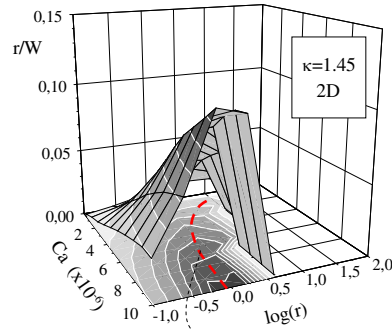


An important result
on SS2φFPM efficiency
(efficiency = lt of oil per kWh spent)
(as indicated by the *DeProF* model)



Energy utilization factor ($f_{EU} = r/W$) & Optimum Operating Conditions (OOC)

$f_{EU} = \{\text{flow rate of oil}\} / \{\text{mechanical power supplied to the system}\}$



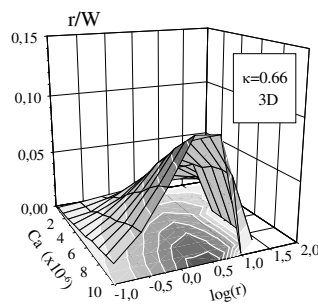
For any $Ca = \text{const}$, **Locus $r^*(Ca)$** : $f_{EU}(Ca, r^*) = \max[f_{EU}(Ca, r)]$

$r^*(Ca) \rightarrow$ Optimum Operating Conditions (OOC)

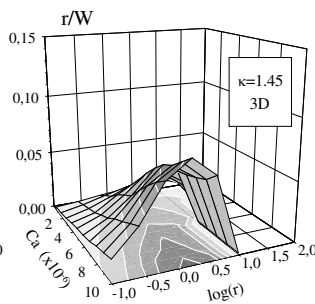


Energy utilization factor ($f_{EU} = r/W$) Effect of viscosity ratio, κ

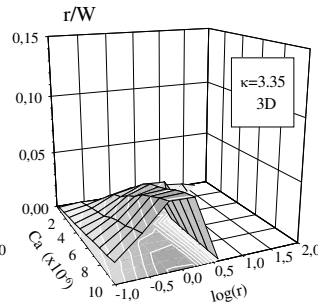
3D



$\kappa=0.66$



$\kappa=1.45$



$\kappa=3.35$

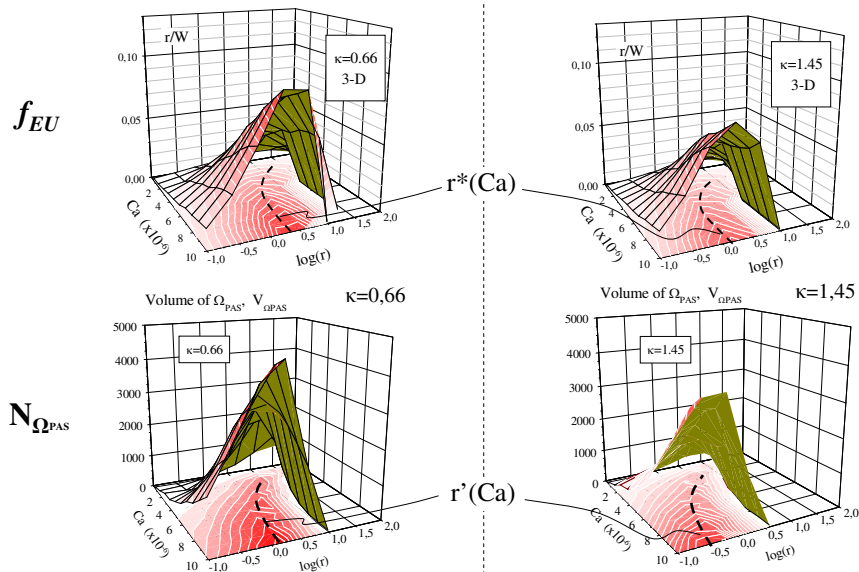
$f_{EU} = \{\text{flow rate of oil}\} / \{\text{mechanical power supplied to the system}\}$



In what way does
process **efficiency**
correlates
to the process **degrees of freedom**?



f_{EU} vs $N_{\Omega_{PAS}}$
 $r^*(Ca)$ vs $r'(Ca)$





Optimum Operating Conds in SS2 ϕ FPM

Q: Are they just a theoretical artifact?

(“contrived” by the *DeProF* model – a “self-fulfilled prophecy”)

A₁: OOC are latent in $k_{rj}(S_w)$ diagrams

look up at experimental works! - latent information!

A₁ → Valavanides, Totaj, ImproDeProF Internal project report

A₂: OOC are justifiable on statistical thermodynamics (the *aSaPP* concept)

A₂ → Valavanides, SPE135429 ATCE2010 (2010),
Daras & Valavanides, MaxEnt2014



OOC in ss2 ϕ fpm: Experimental Verification (Reveal of latent experimental evidence)



Retrospective examination of rel-perm diagrams

Core plug type	Lab measurements (runs)
Berea sandstone	39
Carbonate core	6
Propanat pack	6
Loudon Core	5
Teflon	3
Virtual cores(*LB simulations)	4
Bentheimer	2
Clashach sandstone	1
Outcrop chalk	2
Glass pore network models	15
In total	83

Viscosity ratio $\kappa = \mu_o / \mu_w$	Lab measurements (runs)
$\kappa < 1$	25
$\kappa > 1$	48
$\kappa \approx 1$	6
undisclosed κ	4
In total	83

Constant Ca runs	43
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Retro-examined rel-perm diagrams

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Details of retrospective rel-perm study users.teiath.gr/marval/ArchIII/retrorelperm.pdf

Free download the SS Rel-Perm Data Transformer users.teiath.gr/marval/ArchIII/relpermtrans.xls.

Your lab study is not included? Join the effort in building a rel-perm Data Base ! —> marval@teiath.gr



Transformation of relative permeability data reveals operational efficiency aspects of SS rel.perm. diagrams

In stationary conds, oil/water flowrate ratio ($= \lambda$, the mobility ratio)

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

Energy utilization factor (“oil flowrate per kW spent”)

$$f_{EU} = \frac{r}{W} = k_{ro} \frac{1}{\kappa(r+1)} = k_{rw} \frac{r}{r+1} = k_{ro} \left(\frac{k_{ro}}{k_{rw}} + \kappa \right)^{-1} \quad (2)$$

where

$\kappa = \mu_o/\mu_w$: oil/water viscosity ratio
 $W \equiv \tilde{W} \tilde{k}_w (\tilde{\gamma}_{ow} Ca)^{-2}$: reduced mech. power dissipation (over equiv. 1ph flow)



Demarcation of ss2 ϕ pm operational efficiency (asymptotic limits)

As $Ca \rightarrow \infty$... the capillary effects $\llll$ viscous effects, therefore

$$OE_{\infty} = \frac{\text{Oil flowrate}}{\text{mechanical power}} = \frac{\tilde{q}_o}{(\tilde{W}_o + \tilde{W}_w) \tilde{A} \Delta \tilde{z}} = \frac{(1 - S_{w\infty}) S_{w\infty}}{(1 - S_{w\infty} + \kappa S_{w\infty})} \frac{\tilde{k}}{Ca \tilde{\gamma}_{ow}} \frac{1}{\Delta \tilde{z}}$$

$$\left. \frac{d(OE_{\infty})}{dS_{w\infty}} \right|_{S_{w\infty}^*} = 0 \Rightarrow (\kappa - 1) S_{w\infty}^{*2} + 2S_{w\infty}^* - 1 = 0 \Rightarrow S_{w\infty}^* = \frac{1}{1 + \sqrt{\kappa}}$$

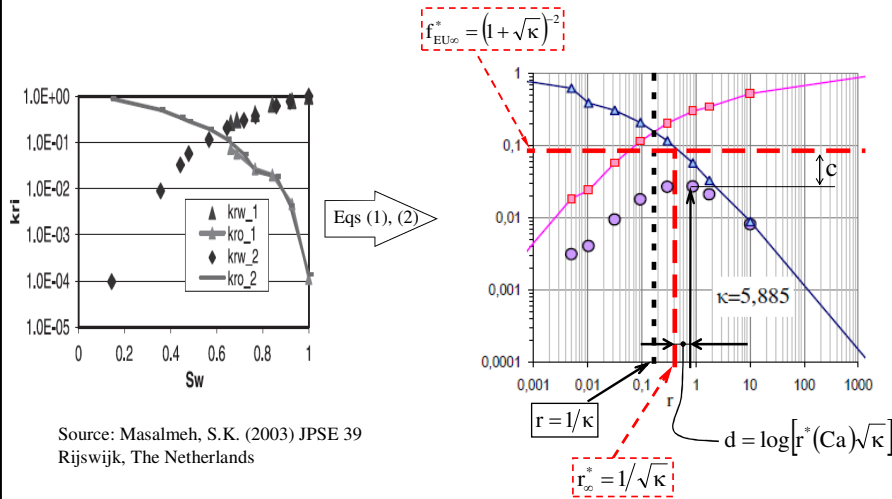
$$\text{Therefore, } r_{\infty}^* = \frac{1}{\kappa} \frac{k_{ro}^*}{k_{rw}^*} r = \frac{1}{\kappa} \frac{S_{ro}^*}{S_{w\infty}^*} = \frac{1}{\kappa} \frac{\frac{\sqrt{\kappa}}{1 + \sqrt{\kappa}}}{\frac{1}{1 + \sqrt{\kappa}}} \Rightarrow \boxed{r_{\infty}^* = 1/\sqrt{\kappa}}$$

and

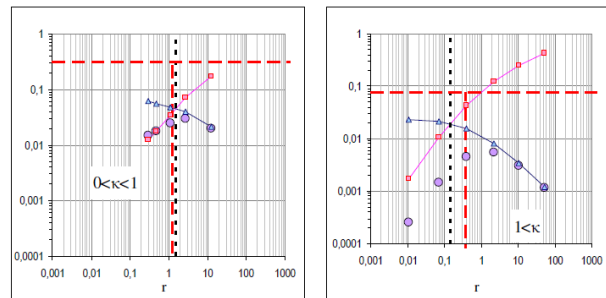
$$\boxed{f_{EU\infty}^* = (1 + \sqrt{\kappa})^{-2}}$$



Typical transformation of rel-perm diagrams



Universal trend of rel-perm diagrams



Set of laboratory data points (recovered from published rel-perm diagrams)

■ k_{ro} , relative permeability of "oil" (non-wetting) ▲ k_{rw} , relative permeability of "water" (wetting)

Data corresponding to k_{ro} , k_{rw} , obtained via transformation, eqs (2)

● $f_{EU} = r/W$, energy utilization coefficient – from eqs(2)

Critical figures from analysis of operational efficiency of steady-state 2-ph flow in p.m.

⋮ $r_c = \frac{1}{\kappa}$ critical flowrate ratio conditions for equality of relperm values

Asymptotic values for pertinent quantities in pure viscous flow conditions, $Ca \rightarrow \infty$

— $r^*_{\infty} = \lim_{Ca \rightarrow \infty} r^* = \frac{1}{\sqrt{\kappa}}$ asymptotic flowrate ratio for optimum operational efficiency

— $f_{EU}(r^*_{\infty}) = \lim_{Ca \rightarrow \infty} f_{EU}(r^*) = \frac{1}{(1 + \sqrt{\kappa})}$ asymptotic limit of locus of optimum operating conditions (OOC)



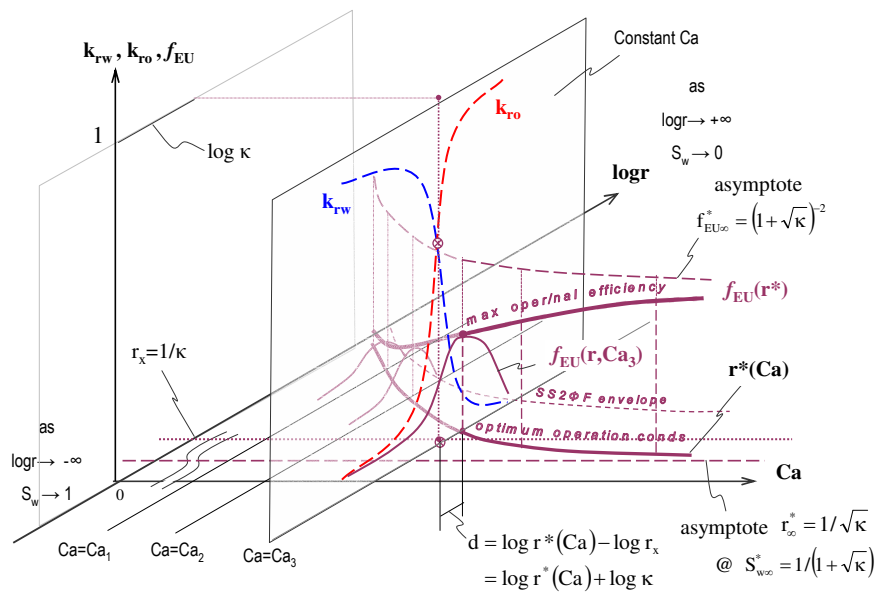
DeProF predictions (mechanistic modeling)
+
Latent experimental evidence (phenomenology)
+
Fractional flow analysis & efficiency demarcation



Universal Operational Efficiency Map



Operational Efficiency Map for ss2φfpm

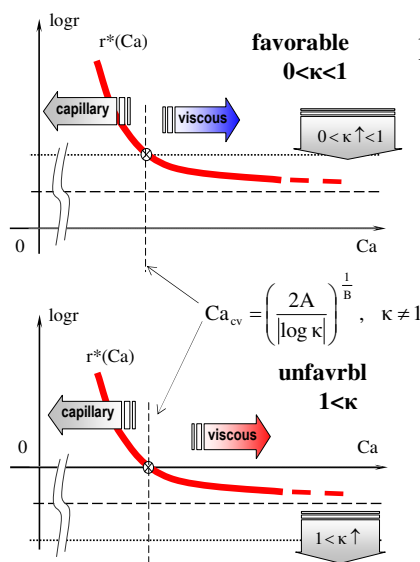




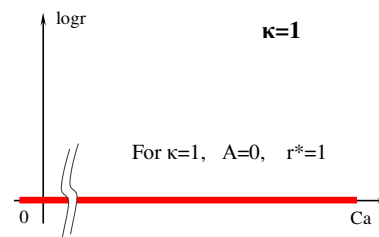
Open Problems



Open Problem 1: Flow characterization



$$\log r^* = -\log \sqrt{\kappa} + \frac{A}{Ca^B}, \quad A, B > 0$$



Implement determine

1. $\kappa=1 \rightarrow B$
2. $\kappa \neq 1 \rightarrow A$
3. $1/\kappa \rightarrow \text{verify } A$



Open Problem 2

Detection of the locus $r^*(Ca)$ of Optimum Operating Conditions

Determination of local max f_{EU}

$$\partial f_{EU} / \partial r |_{r=r^*} = 0 \Rightarrow k_{ro}^* = C_o(Ca)(r^* + 1)$$

$$\partial f_{EU} / \partial r |_{r=r^*} = 0 \Rightarrow k_{rw}^* = C_w(Ca)(r^* + 1)/r^*$$

Integration “constants”, are functions of Ca , related as

$$C_o(Ca) = \kappa C_w(Ca)$$

To detect OptOpConds [locus $r^*(Ca)$ of max f_{EU}],

we need to **resolve the functional form $C_o(Ca)$** [or $C_w(Ca)$]



Open Problem 3

OOC in ss2 ϕ fpm

Justification on the basis of statistical thermodynamics (maximum entropy production principle)

Valavanides, SPE135429, ATCE 2010



Statistical Thermodynamics aspects of ss2φfpm efficiency

ss2φfpm is a stationary, off equilibrium process
provide energy to keep it stationary at fixed operating conditions

*The efficiency of a stationary process in dynamic equilibrium,
is proportional to its spontaneity**

$$\{process\ efficiency\}_{op\ constr} \uparrow \rightarrow \{process\ spontaneity\} \uparrow \text{ or } \{irreversibility\} \downarrow$$

$$\{spontaneity\} \equiv \{irreversibility\}^{-1} \approx \{\text{entropy produced globally}\}$$

The physical domains in which ss2φfpm takes place (to account for entropy production)

{System}:	the porous medium and the two fluids
{Surroundings}:	the heat reservoir in which the {System} resides at constant temperature
{Universe}:	{System} + {Surroundings}

* Atkins 1984 "The Second Law", Freeman ISBN 0-7167-5004-X



Identification of Sources of Entropy

In the sought process (immiscible two-phase flow in porous media),
entropy is present in different scales:

Molecular level (bulk & interfaces) → thermal entropy → Q/T
Q: energy released to the environment (or "dissipated" as "heat") at
temperature T

Core/Field - level → configurational entropy → $k \ln W$
W: number of microstates freely & equiprobably attained
k: Boltzmann-type constant for the particular process

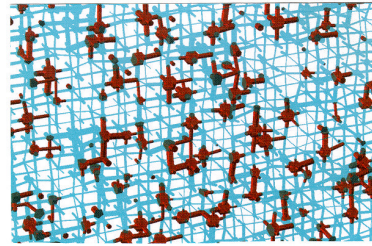
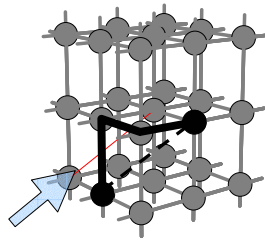


Configurational Entropy (1)

Identification of Microstates

Identification of two complementary domains:

- 1) frontal area perpendicular to macroscopic flow for the connected-oil pathway flow (CPF) / “balls-in-boxes” problem
- 2) reference volume for the disconnected-oil flow (GD+DTF) / “chains-in-barbs” problem



Constantinides & Payatakes, *Transport in Porous Media*, **38** (2000)



Configurational Entropy (2)

Estimation of Number of Microstates

Combinatorics

$$\begin{aligned}
 P' &= P_{\text{COP}} \times P_{\text{DOF}} \\
 &= P_{\text{COP}} \times (P_{\text{DOF1}} \times P_{\text{DOF2}}) \\
 &= \frac{K_{\text{CP}}!}{N_{\text{COP}}!(K_{\text{CP}} - N_{\text{COP}})!} \times \left(\frac{(N_{\text{DTF}} + N_{\text{C}})!}{N_{\text{DTF}}!N_{\text{C}}!} \times \frac{N_{\text{C}}!}{\prod_{i=1}^{I_{\text{max}}} (N_i!)} \right) \\
 &\quad \text{N}_{\text{COP}} \text{ balls-in-} K_{\text{CP}} \text{ boxes} \quad \quad \quad \text{N}_i \text{ chains-in-} (N_{\text{DTF}} + N_{\text{C}}) \text{ barbs}
 \end{aligned}$$



Configurational Entropy (3)

Estimation of Number of Microstates

application of **Stirling's approximation** limiting procedure

$$P' = P_{\text{COP}} \times P_{\text{DOF}} = \frac{K_{\text{CP}}!}{N_{\text{COP}}!(K_{\text{CP}} - N_{\text{COP}})!} \times \frac{(N_{\text{DTF}} + N_{\text{C}})!}{N_{\text{DTF}}!} \frac{1}{\prod_{i=1}^{I_{\text{max}}} (N_i!)}$$

$$\begin{aligned} \ln P' &= \ln(K_{\text{CP}}!) - \ln(N_{\text{COP}}!) - \ln((K_{\text{CP}} - N_{\text{COP}})!) \\ &\quad + \ln[(N_{\text{DTF}} + N_{\text{C}})!] - \ln(N_{\text{DTF}}!) - \sum_{j=1}^{I_{\text{max}}} \ln(N_j!) \end{aligned}$$

$$\boxed{\ln(n!) \cong n \ln(n) - n}$$

$$\begin{aligned} \ln P' &= K_{\text{CP}} \ln K_{\text{CP}} - N_{\text{COP}} \ln N_{\text{COP}} - (K_{\text{CP}} - N_{\text{COP}}) \ln(K_{\text{CP}} - N_{\text{COP}}) \\ &\quad + (N_{\text{DTF}} + N_{\text{C}}) \ln(N_{\text{DTF}} + N_{\text{C}}) - N_{\text{DTF}} \ln N_{\text{DTF}} - \sum_{i=1}^{I_{\text{max}}} N_i \ln(N_i) \end{aligned}$$



Configurational Entropy (4)

Estimation of Number of Microstates

Separation between extensive & intensive contributions

$$\begin{aligned} \ln P' &= K_{\text{CP}} [-\beta \ln \beta - (1 - \beta) \ln(1 - \beta)] \\ &\quad + M(1 - \beta) \left[-(1 - \omega) \ln(1 - \omega) - \left(\omega \ln \omega - \omega \sum_{i=1}^{I_{\text{max}}} n_i^G \ln n_i^G \right) \right] \end{aligned}$$

If no CPF ($\beta=0$)

$$\ln P' = M(1 - \beta) \left[-(1 - \omega) \ln(1 - \omega) - \left(\omega \ln \omega - \omega \sum_{i=1}^{I_{\text{max}}} n_i^G \ln n_i^G \right) \right]$$

And if disconnected oil in singlets

$$\ln P' = M [-(1 - \omega) \ln(1 - \omega) - \omega \ln \omega]$$



CONCLUSIONS

- Two-phase flow in p.m. is “burdened”:
 - with oil disconnection and capillarity effects that restrain or inhibit -to a certain extent- the superficial transport of o & w
 - the bulk phase viscosities of oil & water.
- Process engineers can take advantage of the natural intrinsic characteristics of 2φ flow in p.m., 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 (order of magnitude benefit in process efficiency)



CONCLUSIONS (cont.)

Metaphorically speaking,

the process designer may trade with the “Daemon” (a.k.a. *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).



General CONCLUSIONS

The **DeProF** theory for steady state two-phase flow in porous media:

- **evolved from coordinated research efforts** (implementing experimental/empirical observations, true-to-mechanism hierarchical modeling & numerical simulations at multiple scales and physical interpretation & experimental verification of simulation predictions)
- **is consistent with the pre-existing theory based on Darcy's fractional flow formulation** (nevertheless, it shows conventional wisdom to be not precisely correct, e.g. water saturation is not an independent variable in the description of steady-state two-phase flow in porous media)
- **shows remarkable specificity** (model predictions are consistent with available empirical knowledge; the modelling provision for a plurality of physically admissible mesoscopic flow configurations, appropriately supported by ergodicity considerations, explains the experimental observation of intrinsically unsteady but time averaged steady-state flow regimes)
- **is tentative and dynamic in allowing for changes as new facts are discovered**



Suggestions

Project Management:

Optimization of project /portfolio scheduling

(Valavanides, 2014, *Procedia-SBS* 119)

Transport:

Efficiency optimization of multi modal transport systems



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ImproDeProF project →
http://users.teiath.gr/marval/ArchIII_en.html



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Thank you!

Hoping, I didn’t shoot the messenger!

Dewar, R. (2009) “Maximum Entropy Production as an Inference Algorithm that Translates Physical Assumptions into Macroscopic Predictions: Don’t Shoot the Messenger” *Entropy* **11**