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SK70 – Signe Kjelstrup

Alex Hansen

09.09.2019

PHYSICAL REVIEW E, VOLUME 65, 056310

Relation between pressure and fractional flow in two-phase flow in porous media

Henning Arendt Knudsen* and Alex Hansen[†]

Department of Physics, Norwegian University of Science and Technology, NTNU, NO-7491 Trondheim, Norway

(Received 20 February 2001; published 16 May 2002)

$$A(\text{Ca}) \frac{dF_{\text{nw}}}{dS_{\text{nw}}} + B(\text{Ca}) = \frac{\Delta P}{\Delta P_{\text{s}}}.$$

Comput Geosci (2009) 13:227–234
DOI 10.1007/s10596-008-9109-7

ORIGINAL PAPER

Towards a thermodynamics of immiscible two-phase steady-state flow in porous media

Alex Hansen · Thomas Ramstad

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Abstract We propose that steady-state two-phase flow in porous media may be described through a formalism closely resembling equilibrium thermodynamics. This leads to a Monte Carlo method that will be highly efficient in studying two-phase flow under steady-state conditions numerically.

That is, the porous medium typically would be prepared containing only one of the fluids. The second fluid, immiscible with the first, would then be pumped into the medium and the invasion patterns recorded. Hence, the focus was on *transients*.

Two-phase flow in porous media is also at the core of a vast range of engineering applications ranging from

> Den 22.10.2010 11:02, skrev Ragnhild Skorpa:
> > Hei
> >
> > Trodde vi ble enige om 16 november på telefonen. 23 november passer
> > dårlig siden det er workshop i beregningskjemi den dagen her i
> > Trondheim, og største delen av gruppa vil være der.
> >
> > I denne sammenhengen håper jeg at du har muligheten til å ta det 16
> > november, ellers må det nesten bli 30 november. Passer det?
> >
> > Vennlig hilsen
> > Ragnhild Skorpa

Multiphase flow in porous media under steady-state conditions: Can we use thermodynamics to describe it?

Alex Hansen
Department of Physics
NTNU

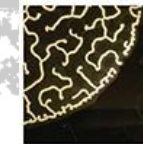
Two immiscible fluids competing for the same pore space in a porous medium undergo instabilities upon instabilities with extremely complex structures as a result. Understanding these structures has value beyond the purely scientific one: some 40 % of the oil in oil reservoirs is deemed unrecoverable due to these structures. The standard approach to this problem has been to study flooding where the porous medium is filled with one of the fluids. The other fluid is then injected and the evolution of the interface between them then followed. An easier situation is, however, to imagine a representative volume element deep inside the porous medium (e.g. the reservoir) and then to follow what happens inside it when a mixture of the fluids is injected into the porous medium at a distance sufficient far away from the representative volume element for local steady state to have set in by the time the fluids reach it. It turns out that this situation has almost been overlooked in the literature. We claim that the structure of the flow under such steady-state conditions is a state in the sense that it only depends on a small set of macroscopic control parameters. Perhaps a "thermodynamics" may be constructed to describe it?

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2010


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 Eur Biophys J (2012) 41:437–448
 DOI 10.1007/s00249-012-0797-5

ORIGINAL PAPER



Kinetic and mesoscopic non-equilibrium description of the Ca^{2+} pump: a comparison

Anders Lervik · Dick Bedeaux · Signe Kjelstrup

 Received: 25 October 2011 / Revised: 31 January 2012 / Accepted: 29 February 2012 / Published online: 28 March 2012
 © European Biophysical Societies' Association 2012

Abstract We analyse the operation of the Ca^{2+} -ATPase ion pump using a kinetic cycle diagram. Using the methodology of Hill, we obtain the cycle fluxes, entropy production and efficiency of the pump. We compare these results with a mesoscopic non-equilibrium description of the pump and show that the kinetic and mesoscopic pictures are in accordance with each other. This gives further support to the mesoscopic theory, which is less restricted and also can include the heat flux as a variable. We also show how motors can be characterised in terms of uni-directional backward fluxes. We proceed to show how the mesoscopic approach can be used to identify fast and slow steps of the model in terms of activation energies, and how this can be used to simplify the kinetic diagram.

Keywords Ca^{2+} -ATPase · Active transport · Ion pump · Kinetic model · Mesoscopic model

Introduction

The lipid bilayers of biological membranes are generally impermeable to ions and most polar molecules (a notable

exception being osmosis of water) and represent a physical barrier to transport (Berg et al. 2002; Nelson 2003). Integral membrane proteins may act as pumps and channels and enable transport of ions and molecules essential for cell operation across the membrane with high selectivity (Berg et al. 2002; Nelson 2003; Garrett and Grisham 2010).

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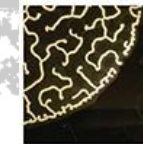
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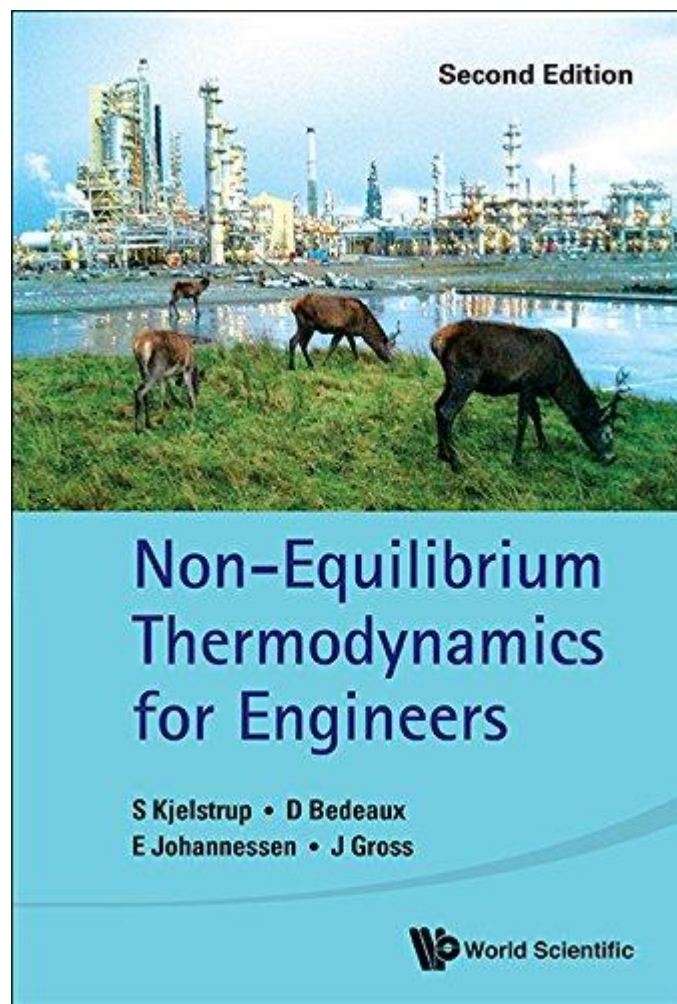
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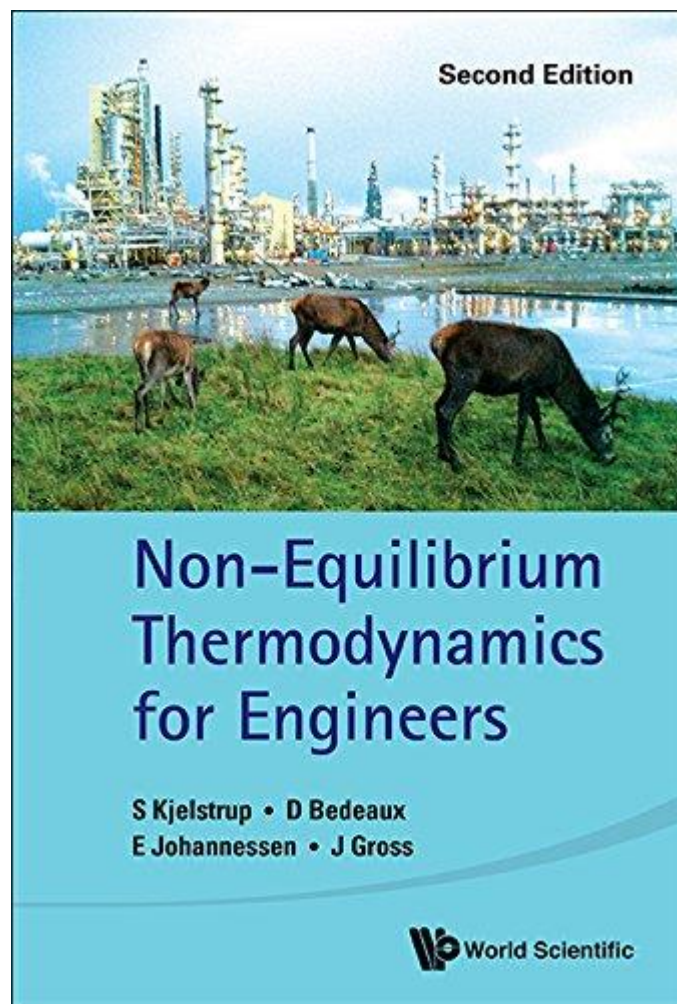
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DICK BEDEAUX AND SIGNE KJELSTRUP

Muscular Contraction and the Calcium Pump

As was shown by Huxley (1953), Huxley & Niedergerke (1954) and Huxley & Hanson (1954), the contraction of skeletal muscles is due to the sliding motion of myosin filaments along actin filaments. The interaction between the filaments is created by cross bridges (Fig. 1) extending from the myosin. According to the theory by Huxley (1969), the heads of the filaments first attach to the actin and then undergo a conformational change whereby the angle of attachment is changed. This then causes a movement of the myosin along the actin. The energy for this process is derived from the hydrolysis of ATP to ADP and inorganic phosphate P_i . ATP binds to the myosin head and hydrolysis takes place. The calcium ions are stored in the sarcoplasmic reticulum, an organelle made for that purpose. When the nerve releases sodium and potassium ions, the surface of the reticulum depolarizes and the calcium ions are released into the sarcoplasm around the muscle fibers (Fig. 2). The calcium then binds to the actin, after which the myosin head also binds to the actin. The ADP and the P_i then detach from the myosin head, which uses the energy for the conformational change to shorten the muscle fibre. When the muscle relaxes, Ca^{2+} -ATPase pumps the calcium ion back to the reticulum, the myosin head detaches from the actin, and ATP binds to the myosin head. (Fig. 3)

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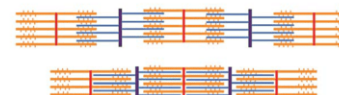


Fig. 1: The top figure illustrates a relaxed muscle fibre and the bottom one a contracted muscle. The orange lines are myosin and the blue lines are actin.

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Non-equilibrium description Comparison

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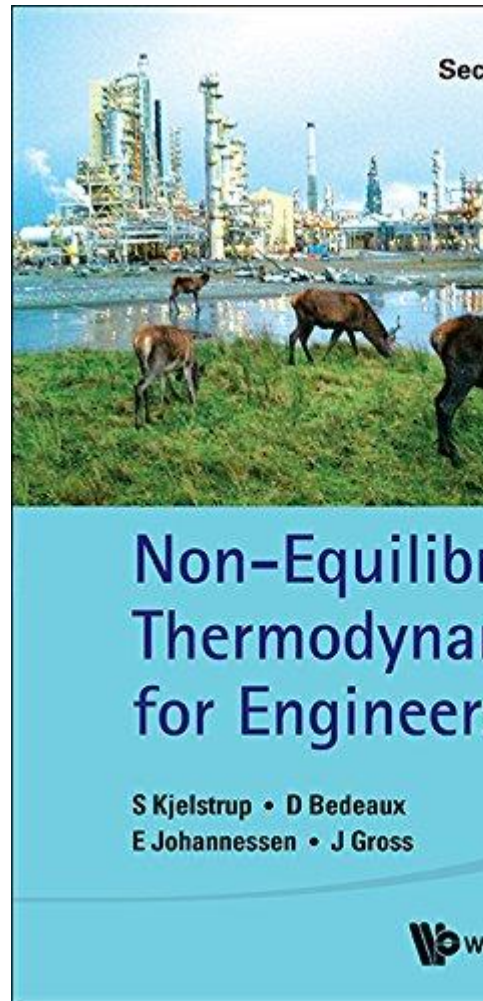
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Contraction and Ion Pump

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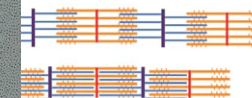
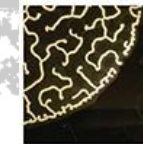


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29

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An Indicator to Evaluate the Thermodynamic Maturity of Industrial Process Units in Industrial Ecology

Anita Zvolinschi and Signe Kjelstrup

Keywords

entropy production
equation balance
energy efficiency
optimization
process units

Summary

The article suggests a measure to evaluate the thermodynamic maturity of industrial systems at the level of single process units. The measure can be quantified with reasonable confidence on the basis of entropy production as defined by irreversible thermodynamics theory. It quantifies, for one process unit, the distance between its actual state of operation and its state with minimum entropy production or optimum energy efficiency, when the two states are constrained with a fixed production capacity of the process unit. We suggest that the minimum entropy production state is a mature state, or that processes that operate at this state are mature. We propose to call the measure "the thermodynamic maturity indicator" (π), and we define it as the ratio between the minimum entropy production and the actual entropy production. We calculated π on the basis of literature data for some examples of industrial process units in the chemical and process industry (i.e., heat exchanger, chemical reactor, distillation column, and paper drying machine). The proposed thermodynamic measure should be of interest for industrial ecology because it emerges from the entropy production rate, a dynamic function that can be optimized and used to understand the thermodynamic limit to improving the energy efficiency of industrial processes. Although not a tool for replacing one process with another or comparing one technology to another, π may be used to assess actual operation states of single process units in industrial ecology.

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Non-Equilibrium Thermodynamics of Heterogeneous Systems

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Summary

The article suggests a measure to evaluate the thermodynamic maturity of industrial systems at the level of single process units. The measure can be quantified with reasonable confidence on the basis of entropy production as defined by irreversible thermodynamics theory. It quantifies, for one process unit, the distance between its actual state of operation and its state with minimum entropy production or optimum energy efficiency, when the two states are constrained with a fixed production capacity of the process unit. We suggest that the minimum entropy production state is a mature state, or that processes that operate at this state are mature. We propose to call the measure "the thermodynamic maturity indicator" (π), and we define it as the ratio between the minimum entropy production and the actual entropy production. We calculated π on the basis of literature data for some examples of industrial process units in the chemical and process industry (i.e., heat exchanger, chemical reactor, distillation column, and paper drying machine). The proposed thermodynamic measure should be of interest for industrial ecology because it emerges from the entropy production rate, a dynamic function that can be optimized and used to understand the thermodynamic limit to improving the energy efficiency of industrial processes. Although not a tool for replacing one process with another or comparing one technology to another, π may be used to assess actual operation states of single process units in industrial ecology.

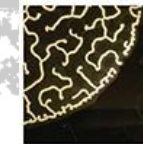
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Journal of Industrial Ecology 159



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 non-equilibrium
 comparison

Kjelstrup

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Series on Advances in Statistical Mechanics – Volume 16

Non-Equilibrium Thermodynamics of Heterogeneous Systems

SIGNE KJELSTRUP DICK BÉDEAUX

World Scientific

 Int. J. of Thermodynamics,
 Vol.7, (No.3), pp.107-114, September 2004

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Application of Irreversible Thermodynamics to Distillation

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Abstract

We compare three different ways of modelling tray distillation to each other, and to experimental data: the most common way that assumes equilibrium between the liquid and vapour phases at the outlets of each tray, and two more precise methods that use irreversible thermodynamics. Irreversible thermodynamics determines the driving forces and fluxes of a system in agreement with the second law. It is shown that the methods using irreversible thermodynamics (Maxwell-Stefan equations) are superior to the method that assumes that equilibrium is reached on each tray. The Soret effect must be included to have a good description of the heat flux.

Keywords: Irreversible Thermodynamics, Distillation, Maxwell-Stefan Equation, Soret/Dufour effects, Interface.

1. Introduction

Distillation is the most common separation method. It accounts for 11 % of the industrial energy demand in the USA in 1991 (Humphrey and Siebert 1992). Since industrial scale experiments are demanding and expensive, distillation models are useful for design of distillation columns. Tray distillation is most commonly modelled by assuming that equilibrium is established between the vapour and the liquid at the outlets of each tray in the column. However, in reality equilibrium is not reached. The first attempt to account for the irreversible nature of the process was to introduce tray efficiencies. The Murphree efficiency measures to which degree equilibrium is reached (King 1980). The Murphree efficiency has been used to describe distillation with some success for binary mixtures at steady state. The method breaks down for multi-component systems or for dynamic behaviour. Moreover, the Murphree efficiency provides no physical explanation for why equilibrium is not reached.

Descriptions that introduce such explanations have their origin in irreversible thermodynamics (Kjølken 1994, Forland et al.

2001, Demirel and Sandler 2001). In irreversible thermodynamics the fluxes and forces of the system are derived in a systematic way. All possible coupling effects can be included, or discarded, within a framework that complies with the second law. The pioneering articles, in that irreversible thermodynamics was applied to distillation, were written by Krishnamurthy and Taylor (1983a, 1983b). These authors modelled distillation by means of driving forces and transfer rates without the assumption of equilibrium between the liquid and the vapor at the outlets of a tray. Interestingly, the authors did not expect the results to be that good at first try. The transfer rates were formulated using Maxwell-Stefan equations, and this approach is therefore called the Maxwell-Stefan approach from now on. Research using this approach is now described in books (Taylor and Krishna 1993, Perry and Green 1997, Seader and Henley 1998) and reviewed by Krishna and Wesselingh (1997). The increased computing capacity and speed has helped to develop the Maxwell-Stefan approach.

Instead of assuming equilibrium between the liquid and vapour at the outlets of each tray, in the Maxwell-Stefan approach one introduces a

Int.J. Thermodynamics, Vol.7 (No.3) 107

*Author to whom correspondence should be addressed

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An Indicator to Evaluate the Thermodynamic Maturity of Industrial Process Units in Industrial Ecology

Anita Zvolinschi and Signe Kjelstrup

Keywords

 entropy production
 equipartition
 energy balance
 energy efficiency
 optimization
 process units

Summary

The article suggests a measure to evaluate the thermodynamic maturity of industrial systems at the level of single process units. The measure can be quantified with reasonable confidence on the basis of entropy production as defined by irreversible thermodynamics theory. It quantifies, for one process unit, the distance between its actual state of operation and its state with minimum entropy production or optimum energy efficiency, when the two states are constrained with a fixed production capacity of the process unit. We suggest that the minimum entropy production state is a mature state, or that processes that operate at this state are mature. We propose to call the measure "the thermodynamic maturity indicator" (π), and we define it as the ratio between the minimum entropy production and the actual entropy production. We calculated π on the basis of literature data for some examples of industrial process units in the chemical and process industry (i.e., heat exchanger, chemical reactor, distillation column, and paper drying machine). The proposed thermodynamic measure should be of interest for industrial ecology because it emerges from the entropy production rate, a dynamic function that can be optimized and used to understand the thermodynamic limit to improving the energy efficiency of industrial processes. Although not a tool for replacing one process with another or comparing one technology to another, π may be used to assess actual operation states of single process units in industrial ecology.

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 Non-equilibrium
 Thermodynamics

Kjelstrup

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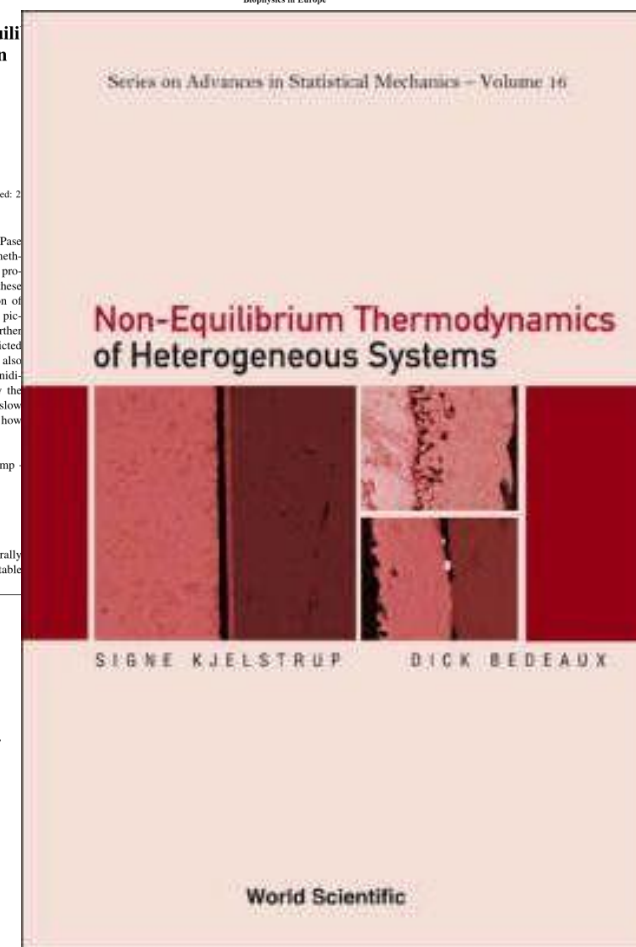
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Efficiency of electrochemical gas compression, pumping and power generation in membranes

 Jacopo Catalano^{a,*}, Anders Bienten^{a,b}, David Nicolas Østedgaard-Munck^a, Signe Kjelstrup^b
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 Electrochemical gas compression
 Power generation
 Electrokinetic

1. Introduction

Electrokinetic effects in porous materials and membranes arise due to the coupling between the movement of ions and solvent. In e.g. water such a coupling can be explained and modelled by electrostatic interactions between charged ions and polar water molecules. Electrokinetic effects can be utilised for direct conversion of potential or kinetic energy (e.g. Pressurised liquids and gases) into electrochemical energy or vice versa [1]. This is potentially attractive for many applications [2] such as microfluidic pumps, gas compressors for cooling cycles, small generators in e.g. domestic compressed air energy storage [3] or heat engines e.g. organic Rankine cycles [4].

The Savién relations have been known since long, but specific studies of electrokinetic energy conversion were done first in the 1960s by Osterle and co-workers [1,5] and Burgeen and Nakache [6,7]. They predicted a maximum first law efficiency (η_{SL}) of the order 1–3% and up to 17%, respectively. During the past decade renewed interest in this topic has emerged, and most reports focus on the transport properties of straight nanochannels with well-defined dimensions [8–23]. Recently [2,24], experimental

values of the electrokinetic figure-of-merit [1,2,24] have shown that efficiency of about 20% can be obtained in commercial Naion membranes and it is increasing with temperature.

Up to now all theoretical studies of electrokinetic energy conversion have only considered incompressible fluids and in particular aqueous solutions. However, gas phase electrokinetic energy conversion is possible too and the potential applications are electrochemical gas compression or power generation (expander). Some experimental works have been reported on electrochemical compression of H_2 through a membrane [25–29], with focus on high pressure liquefaction of H_2 . Electrochemical gas compression in membranes for cooling applications is described in the patent literature, e.g. Refs. [30–32]. None of the patents disclose technical details or theoretical considerations with respect to e.g. efficiency and power density.

Fig. 1 gives a schematic illustration of electro-osmosis with liquid (left) and gas reservoirs (right). In the first case, an ion, say Li^+ , migrates through the membrane due to an external electric potential (ϕ) difference. Each Li^+ couples with a number of water molecules, that are quantified by the water transport number (t_w). In popular terms one may say that Li^+ is dragging or pumping water through the membrane as it is moving in the electric field.

Alternatively, a gas phase can supply the conducting ion by gas oxidation and subsequent reduction on the two membrane sides.

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 3), pp.107–114, September-2004

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Application of Irreversible Thermodynamics to Distillation

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Distillation is a process that introduces some nonequilibrium. The origin of nonequilibrium is the irreversible thermodynamics (Kjelstrup 1994, Forland et al.

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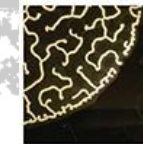
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SIGNE KJELSTRUP DICK BÉDEAUX

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Efficiency of electrochemical gas compression, pumping and power generation in membranes

 Jacopo Catalano^a, Anders Bentzen^b
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^b Department of Chemistry, Norwegian University of Science and Technology, Norway

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...and lots and lots more...

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29

World Scientific

PHYSICAL REVIEW E **87**, 025001 (2013)

Effective rheology of bubbles moving in a capillary tube

Santanu Sinha,^{1,*} Alex Hansen,^{1,†} Dick Bedeaux,^{2,‡} and Signe Kjelstrup^{2,§}

¹*Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway*

²*Department of Chemistry, Norwegian University of Science and Technology, N-7491 Trondheim, Norway*

(Received 4 September 2012; published 14 February 2013)

2015



2017



Dealing with thermodynamics

Perhaps, after all, the wise man's attitude towards thermodynamics should be to have *nothing to do with it*. To deal with thermodynamics is to look for trouble. This is not the citation of a famous scientist, but the result of a deep cogitation following mere observations. Why do we need to get involved in a field of knowledge which, within the last hundred years, has exhibited the largest number of schizophrenics and megalomaniacs, imbalanced scientists, paranoiacs, egocentrists, and probably insomniacs and sleepwalkers?

Gérard A. Maugin,
The Thermodynamics of Nonlinear Irreversible Behaviors
(World Scientific, Singapore, 1999)

Three Laws of Thermodynamics

1. $dE = T dS + dW.$
2. $dS \geq 0.$
3. $S \rightarrow 0$ as $T \rightarrow 0.$

Three Laws of Thermodynamics

1. You cannot win.
2. You cannot break even.
3. You cannot leave the game.

Transp Porous Med (2017) 116:869–888
DOI 10.1007/s11242-016-0804-x



A Monte Carlo Algorithm for Immiscible Two-Phase Flow in Porous Media

**Isha Savani¹ · Santanu Sinha² · Alex Hansen² ·
Dick Bedeaux³ · Signe Kjelstrup³ · Morten Vassvik¹**

Transp. Porous Media **116**, 869 (2017)

Non-isothermal Transport of Multi-phase Fluids in Porous Media. The Entropy Production

Signe Kjelstrup^{1}, Dick Bedeaux¹, Alex Hansen², Bjørn Hafskjold¹ and Olav Galteland¹*

¹ PoreLab, Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway, ² PoreLab, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Frontiers in Physics **6**, 126 (2018)


Non-isothermal Transport of Multi-phase Fluids in Porous Media. Constitutive Equations

Signe Kjelstrup^{1}, Dick Bedeaux¹, Alex Hansen², Bjørn Hafskjold¹ and Olav Galteland¹*

¹ PoreLab, Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway, ² PoreLab, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Frontiers in Physics **6**, 150 (2019)

Relations Between Seepage Velocities in Immiscible, Incompressible Two-Phase Flow in Porous Media

Alex Hansen¹  · Santanu Sinha² · Dick Bedeaux³ · Signe Kjelstrup³ · Magnus Aa. Gjennestad¹ · Morten Vassvik¹

Transport in Porous Media, **125**, 565 (2018)

Core idea of thermodynamics:
Euler homogeneous functions and energy conservation

Core idea of thermodynamics:
Euler homogeneous functions and energy conservation

$$\mathbf{v}_w = \mathbf{v} + S_n(\mathbf{v}' - \mathbf{v}_m)$$

$$\mathbf{v}_n = \mathbf{v} - S_w(\mathbf{v}' - \mathbf{v}_m)$$

$$\mathbf{v}_w = \mathbf{v} + S_n(\mathbf{v}' - \mathbf{v}_m)$$

$$\mathbf{v}_n = \mathbf{v} - S_w(\mathbf{v}' - \mathbf{v}_m)$$

Co-moving velocity

Mass conservation

$$\mathbf{v}_w = \mathbf{v} + S_n(\mathbf{v}' - \mathbf{v}_m)$$

$$\mathbf{v}_n = \mathbf{v} - S_w(\mathbf{v}' - \mathbf{v}_m)$$

Mass conservation

$$\frac{\partial S_w}{\partial t} + \nabla \cdot \mathbf{v}_w S_w = 0$$

$$\frac{\partial S_n}{\partial t} + \nabla \cdot \mathbf{v}_n S_w = 0$$

$$\mathbf{v}_w = \mathbf{v} + S_n(\mathbf{v}' - \mathbf{v}_m)$$

$$\mathbf{v}_n = \mathbf{v} - S_w(\mathbf{v}' - \mathbf{v}_m)$$

Mass conservation

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$$\mathbf{v}_n = \mathbf{v} - S_w(\mathbf{v}' - \mathbf{v}_m)$$

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial S_w}{\partial t} + \nabla \cdot [\mathbf{v} + (1 - S_w)(\mathbf{v}' - \mathbf{v}_m)] S_w = 0$$

$$\frac{\partial S_w}{\partial t} + \nabla \cdot \mathbf{v}_w S_w = 0$$

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$$\nabla \cdot \mathbf{v} = 0$$

Constitutive Equations

$$\frac{\partial S_w}{\partial t} + \nabla \cdot [\mathbf{v} + (1 - S_w)(\mathbf{v}' - \mathbf{v}_m)] S_w = 0$$

Constitutive equations

$$\nabla \cdot \mathbf{v} = 0$$

$$\mathbf{v} = -\tilde{M}(S_w, \mu_w, \mu_n, Ca) \nabla P - \tilde{N}(S_w, \mu_w, \mu_n, Ca) \nabla S_w$$

$$\mathbf{v} = -\tilde{M}(S_w, \mu_w, \mu_n, Ca) \nabla P - \tilde{N}(S_w, \mu_w, \mu_n, Ca) \nabla S_w$$

$$\tilde{N}(S_w, \mu_w, \mu_n, Ca) = M_P(S_w, \mu_w, \mu_n, Ca) \frac{dP_c}{dS_w}$$

$$\mathbf{v} = -\tilde{M}(S_w, \mu_w, \mu_n, Ca) \nabla P - \tilde{N}(S_w, \mu_w, \mu_n, Ca) \nabla S_w$$

$$\tilde{N}(S_w, \mu_w, \mu_n, Ca) = M_P(S_w, \mu_w, \mu_n, Ca) \frac{dP_c}{dS_w}$$

$$\mathbf{v} = -\tilde{M}(S_w, \mu_w, \mu_n, Ca) \nabla (P - P_c)$$

$$\mathbf{v}_m = -\tilde{B} \nabla (P - P_c) + \tilde{M} \frac{d^2 P_c}{dS_w^2} \nabla S_w$$

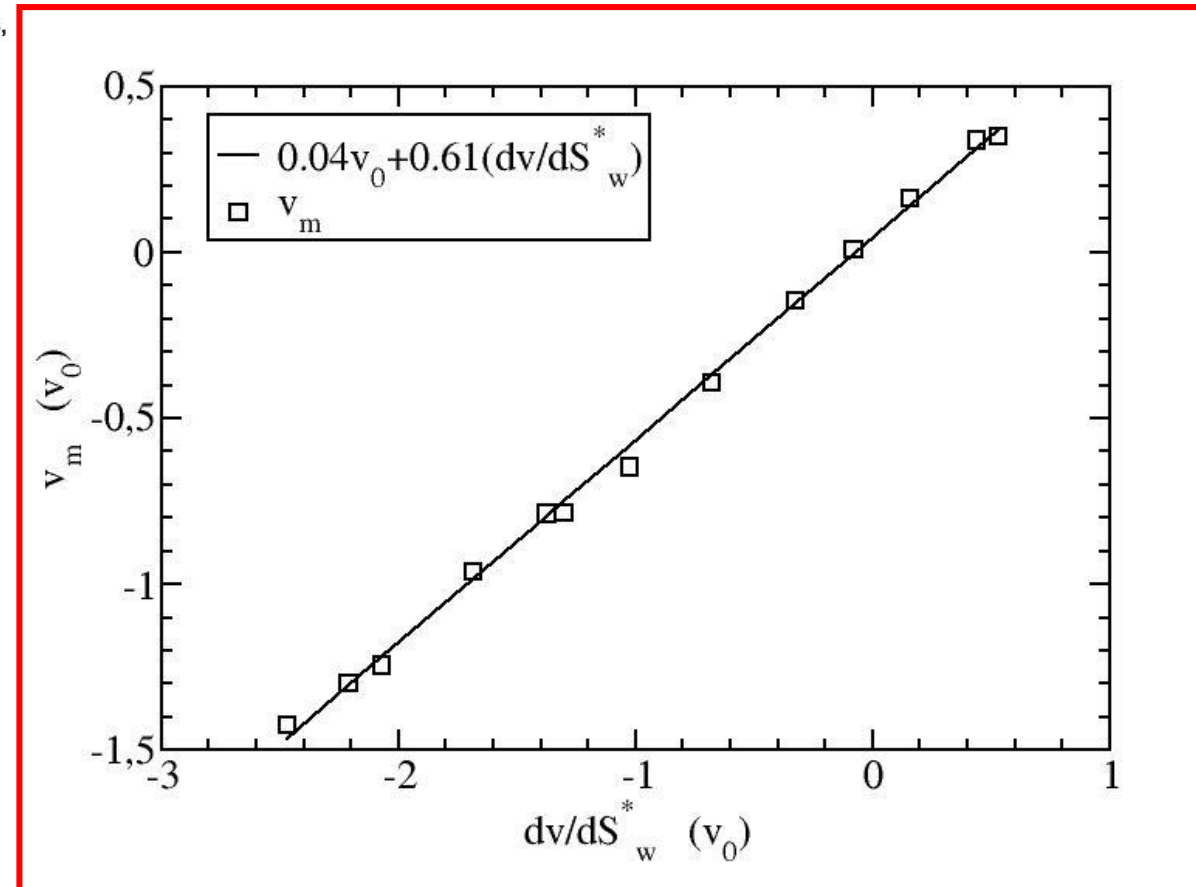
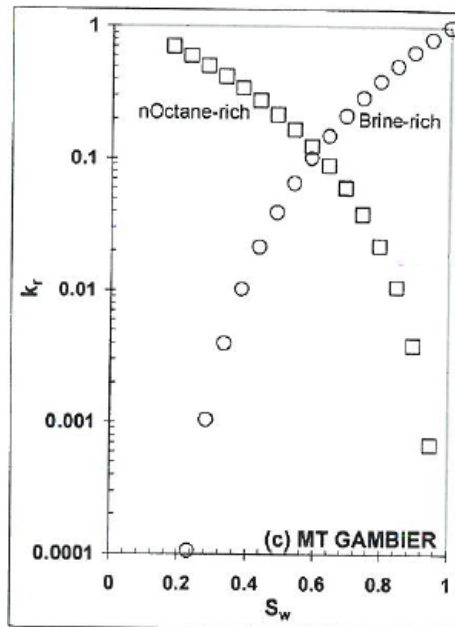
SPE 113386

Capillary Pressure and Relative Permeability of Small Cores

O. A. Olafuyi, SPE, University of New South Wales, Y. Cinar, SPE, University of New South Wales, M.A. Knackstedt, SPE, Australian National University, and W.V. Pinczewski, SPE, University of New South Wales

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This paper was prepared for presentation at the 2008 SPE/DOE Improved Oil Recovery Symposium held in Tulsa, Oklahoma, U.S.A., 19–23 April 2008.



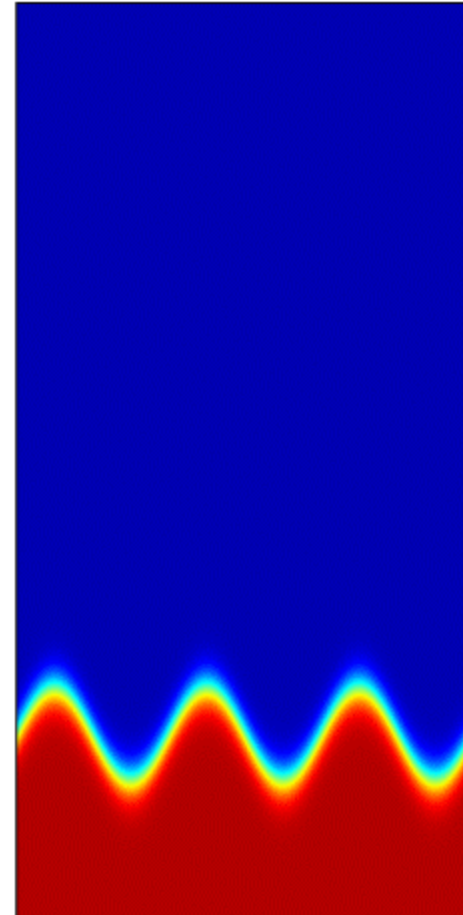
$$\mathbf{v}_m = -\tilde{B} \nabla (P - P_c) + \tilde{M} \frac{d^2 P_c}{dS_w^2} \nabla S_w$$

Where relative permeability is ok.

$$\tilde{B} = a \frac{k}{\mu_w} + b \frac{d\tilde{M}}{dS_w}$$

Immiscible Two-Phase Flow

Imbibition

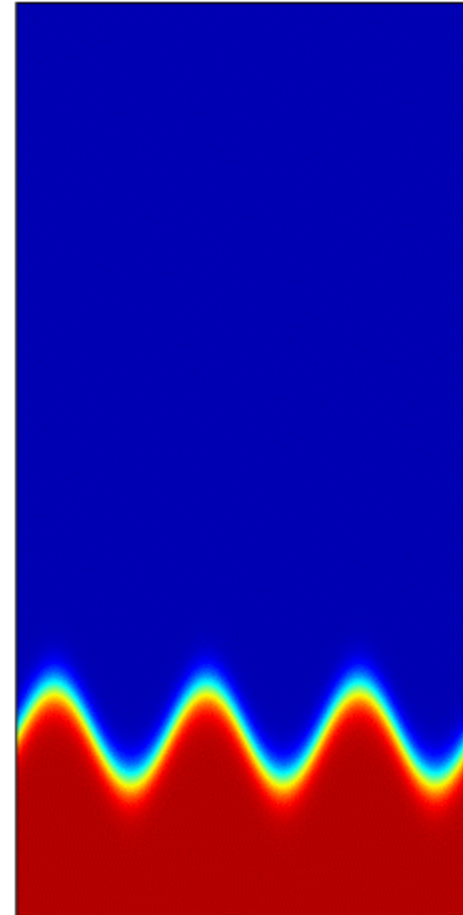


Non-wetting fluid

Wetting fluid

Immiscible Two-Phase Flow

Imbibition

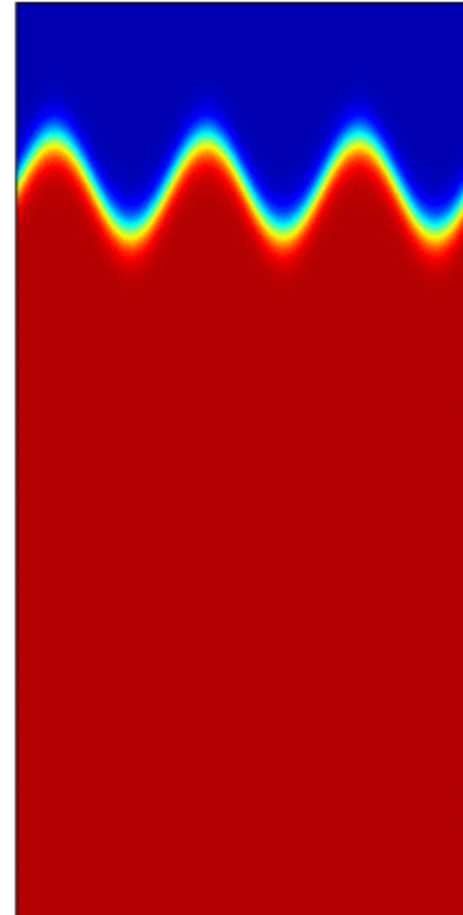


Non-wetting fluid

Wetting fluid

Immiscible Two-Phase Flow

Drainage

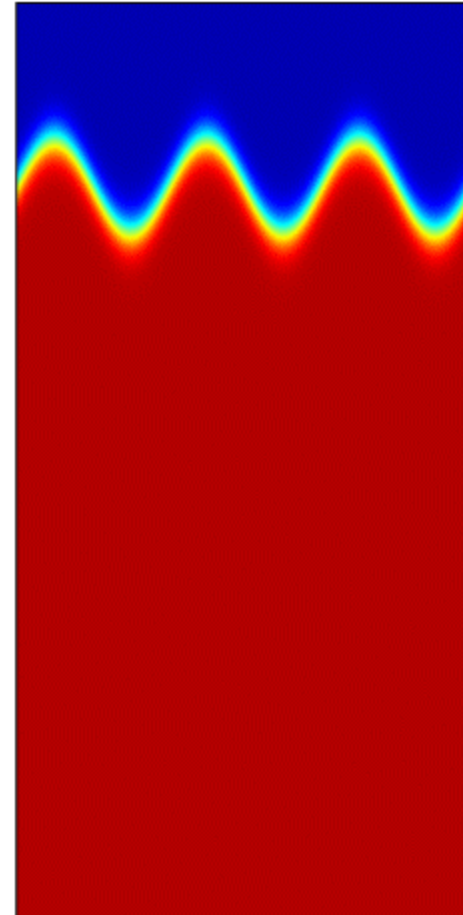


Non-wetting fluid

Wetting fluid

Immiscible Two-Phase Flow

Drainage



Non-wetting fluid

Wetting fluid



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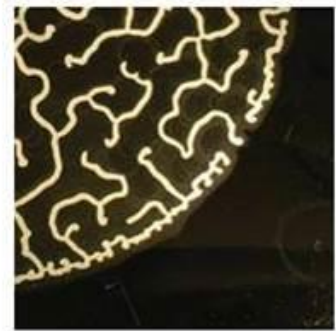
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