SK70 – Signe Kjelstrup

Alex Hansen

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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)

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

2008

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

Received: 5 May 2008 / Accepted: 4 September 2008 / Published online: 1 October 2008

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

2010

> 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?

PoreLab
NTNU-UiO Porous Media Laboratory

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

ORIGINAL PAPER

EBSA
Biophysics in Europe

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

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 unidirectional 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).

Among the transporting integral membrane proteins are the P-type ATPases, which actively transport cations across biological membranes. The P-type ATPases constitute a large family of membrane proteins including the Ca^{2+}-ATPase, the Na^{+}/K^{+}-ATPase, the plant and fungal H^{+}-ATPases and the heavy-metal-transporting ATPases (Møller et al. 2010; Kühlbrandt 2004; Lee and East 2001). The sarcoplasmic reticulum Ca^{2+}-ATPase (SERCA) was the first of the P-type ATPases for which a 3D structure was determined by Toyoshima et al. (2000). The structure of the Ca^{2+}-ATPase in one of its conformations is shown in Fig. 1. Since the first 3D structure was reported, several other conformations[1] of Ca^{2+}-ATPase have also been resolved (Xu et al. 2002; Toyoshima and Nomura 2002; Sørensen et al. 2004; Olesen et al. 2004, 2007a; Toyoshima and Mizutani 2004; Toyoshima et al. 2004, 2007, 2011; Obara et al. 2005; Søhoel et al. 2006; Jensen et al. 2006; Moncoq et al. 2007; Takahashi et al. 2007; Laursen et al. 2009; Winther et al. 2010), enabling a structural interpretation of the operation of the pump. Combined with the vast experimental kinetic and mutagenic data available for the Ca^{2+}-ATPase, this has led to a detailed picture of the

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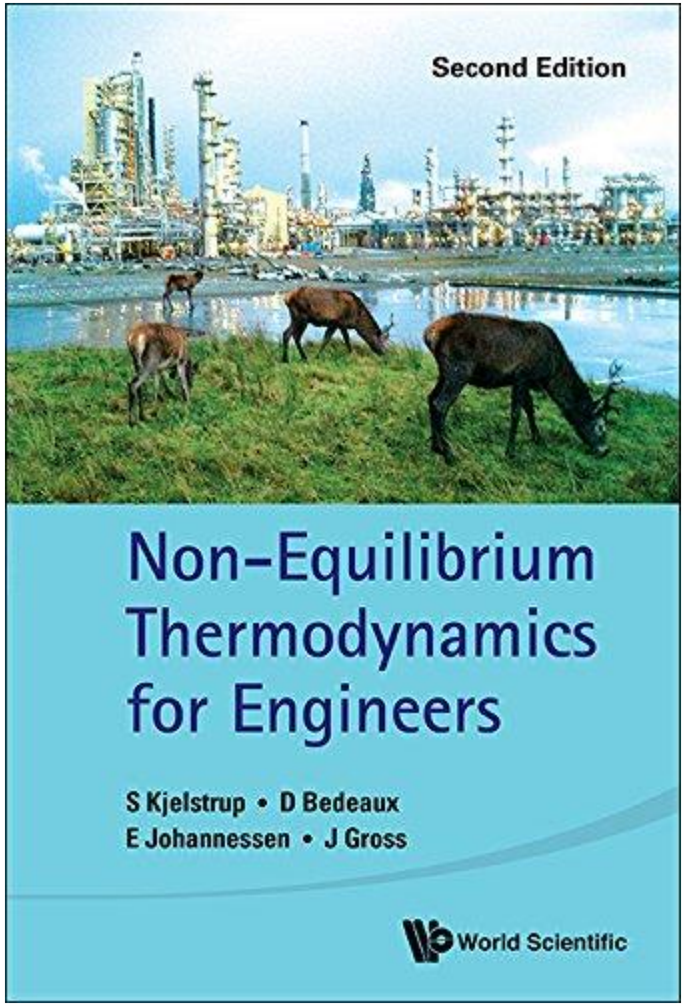

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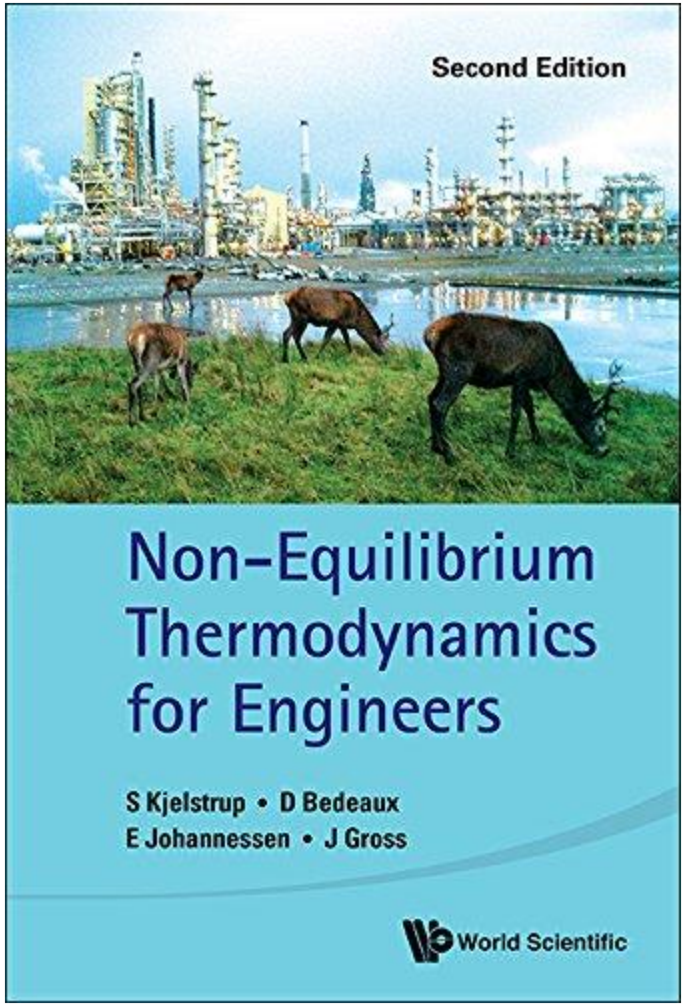

DICK BEDEAUX AND SIGNE KJELSTRUP

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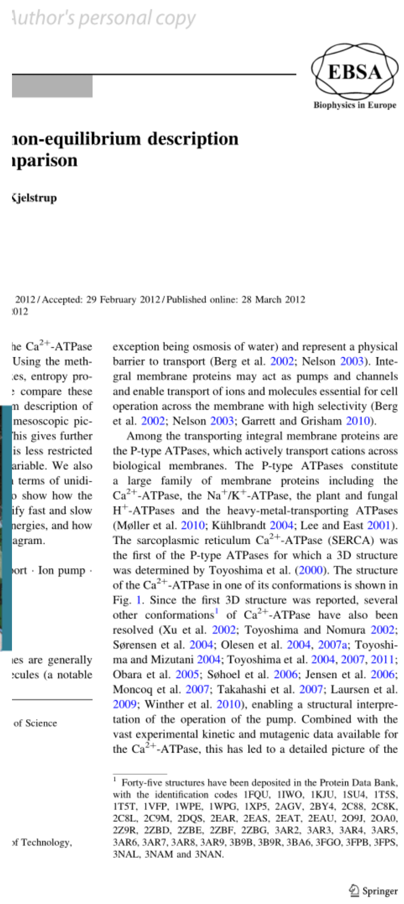
Fig. 1: The top figure illustrates a relaxed muscle fibre and the bottom one a contracted muscle. The orange lines are myosin and the blue lines are actin.



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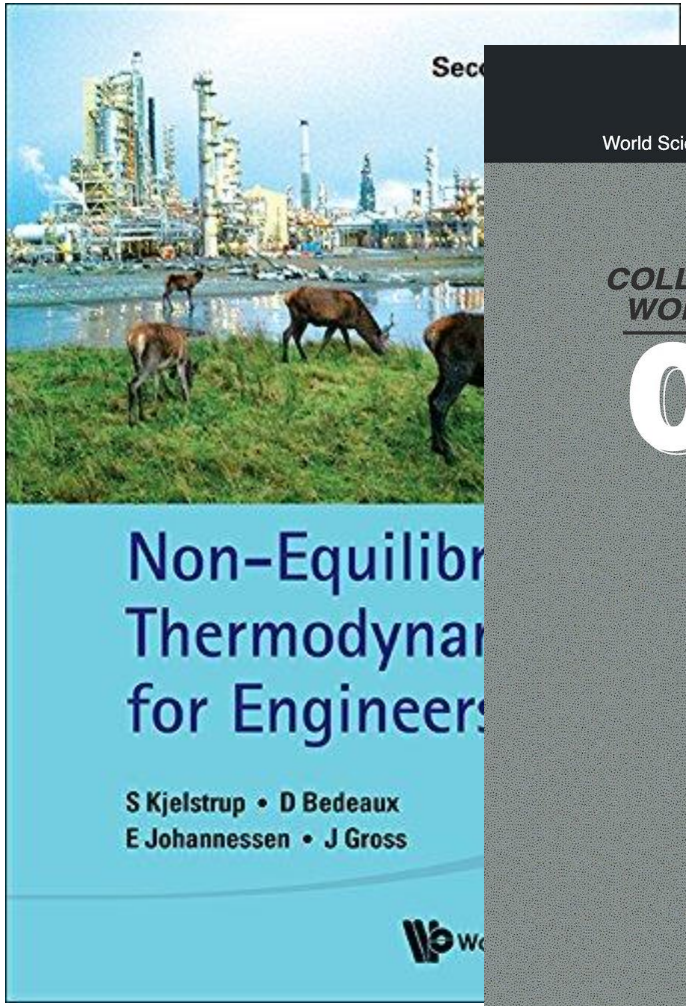
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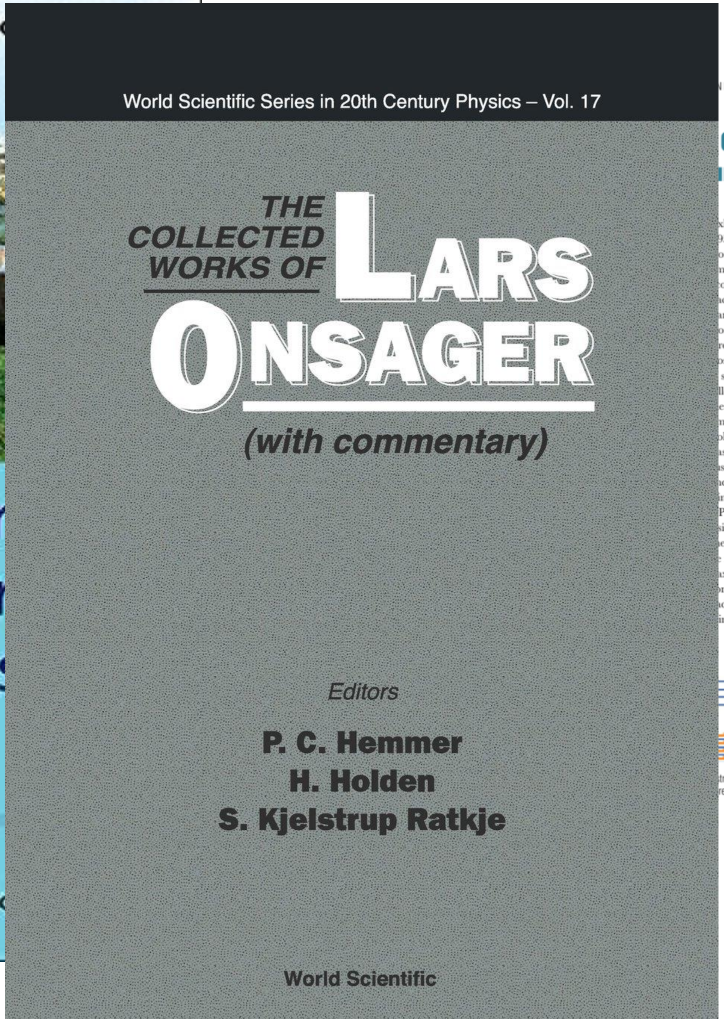
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Contraction and
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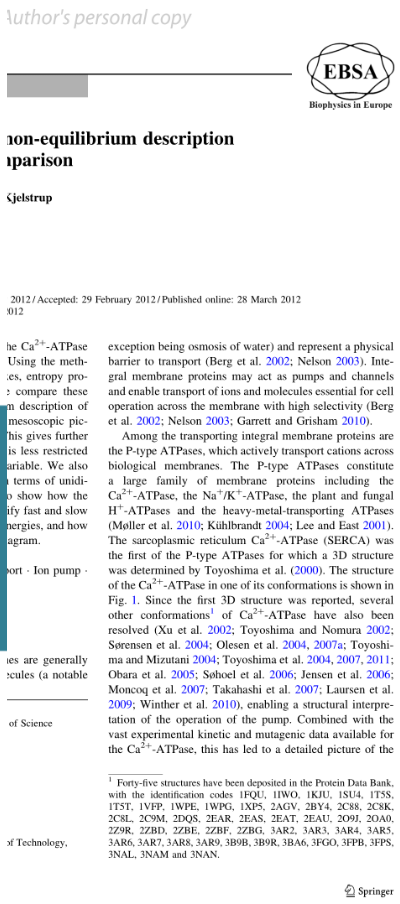
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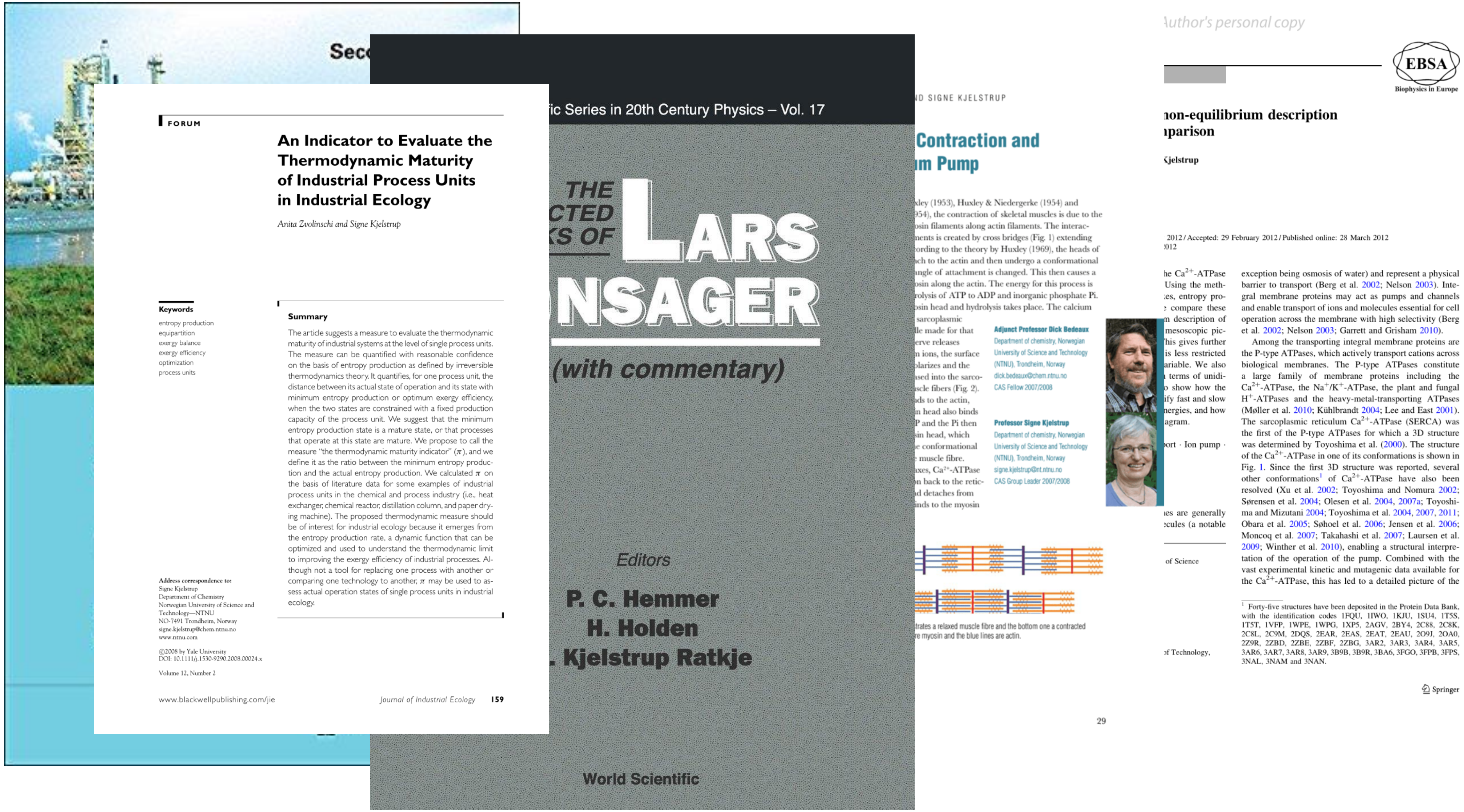

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An Indicator to Evaluate the Thermodynamic Maturity of Industrial Process Units in Industrial Ecology

Anita Zvolinschi and Signe Kjelstrup

Keywords
entropy production
equipartition
exergy balance
exergy 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 exergy 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 exergy 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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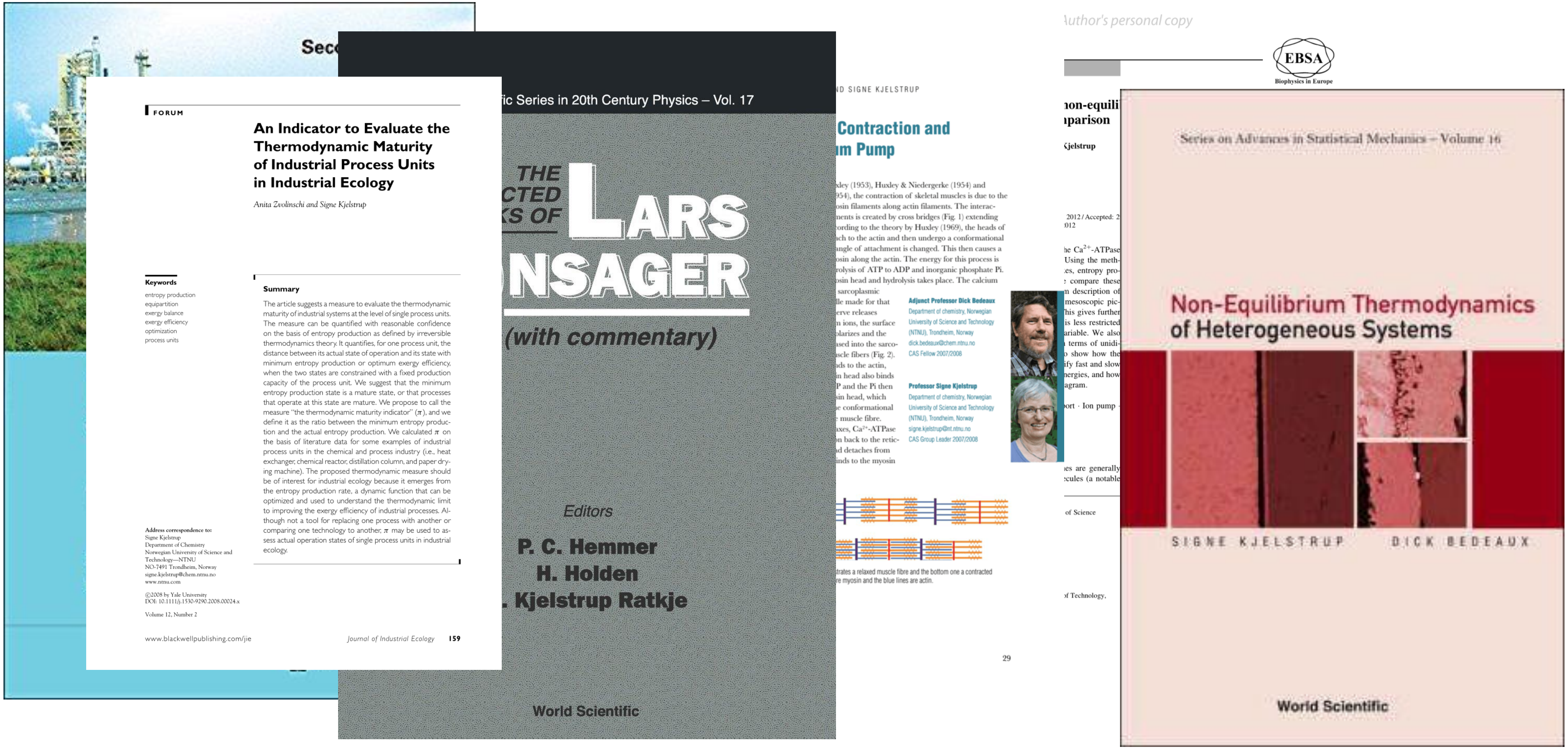
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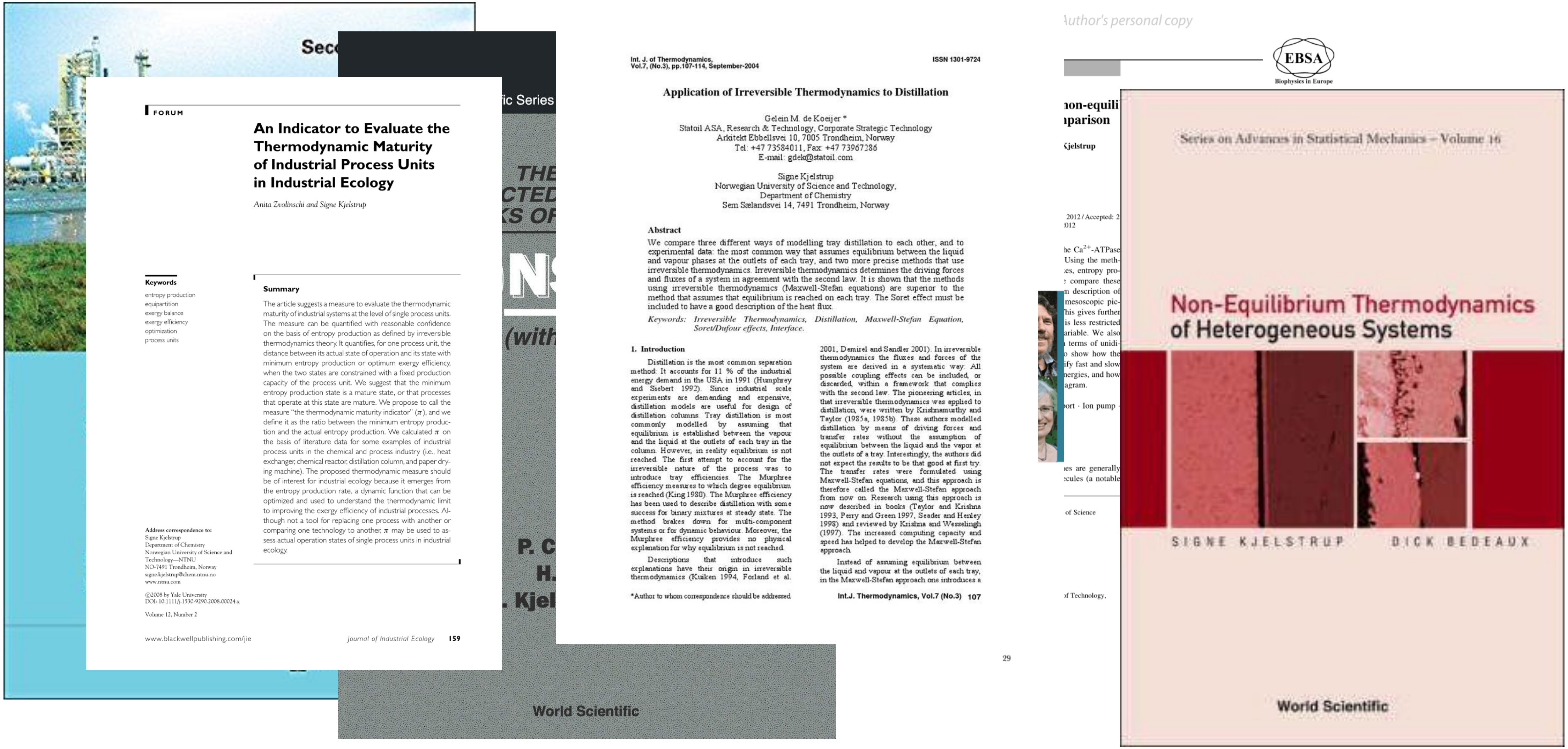

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Application of Irreversible Thermodynamics to Distillation

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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 brakes 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 (Kuiken 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 (1985a, 1985b). 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

*Author to whom correspondence should be addressed

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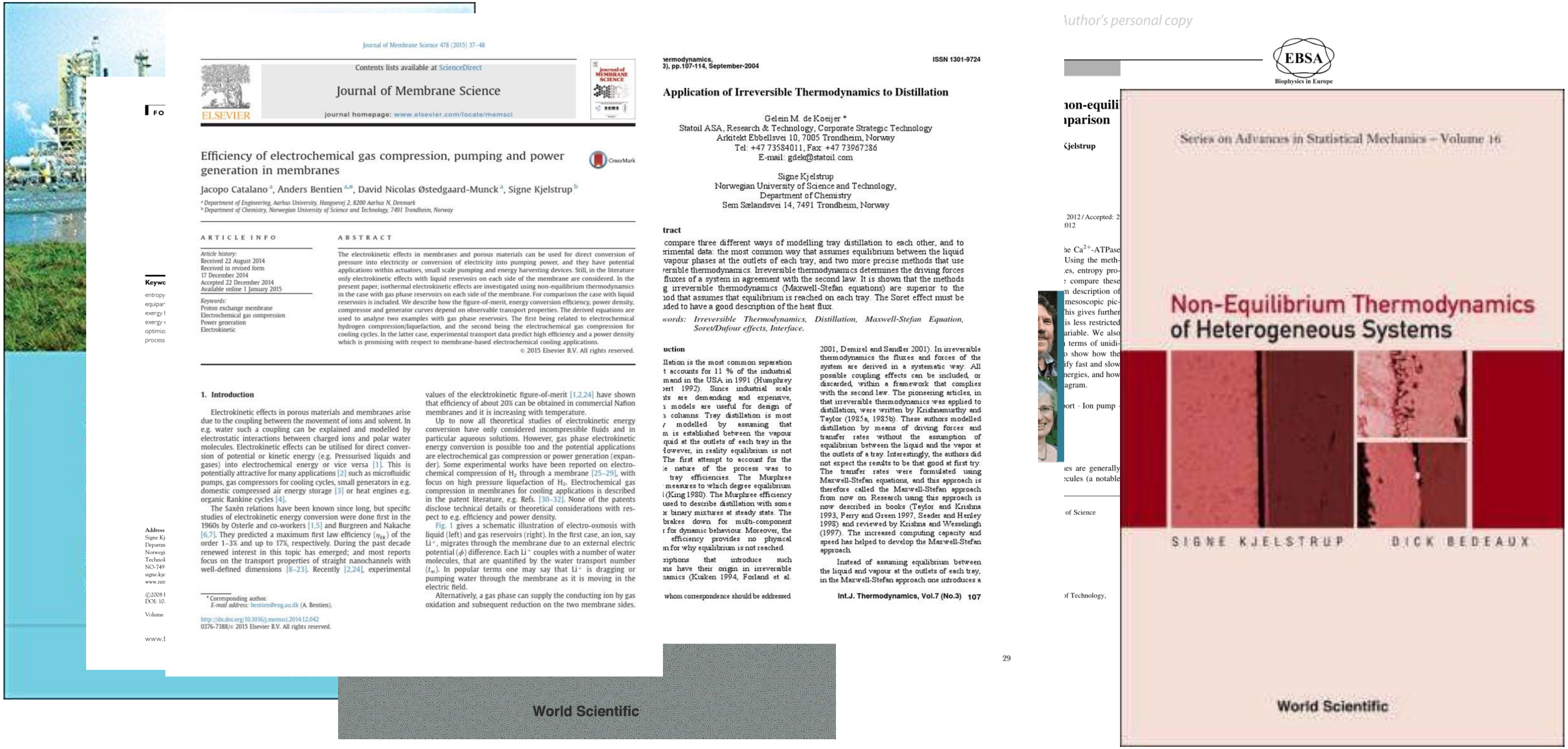
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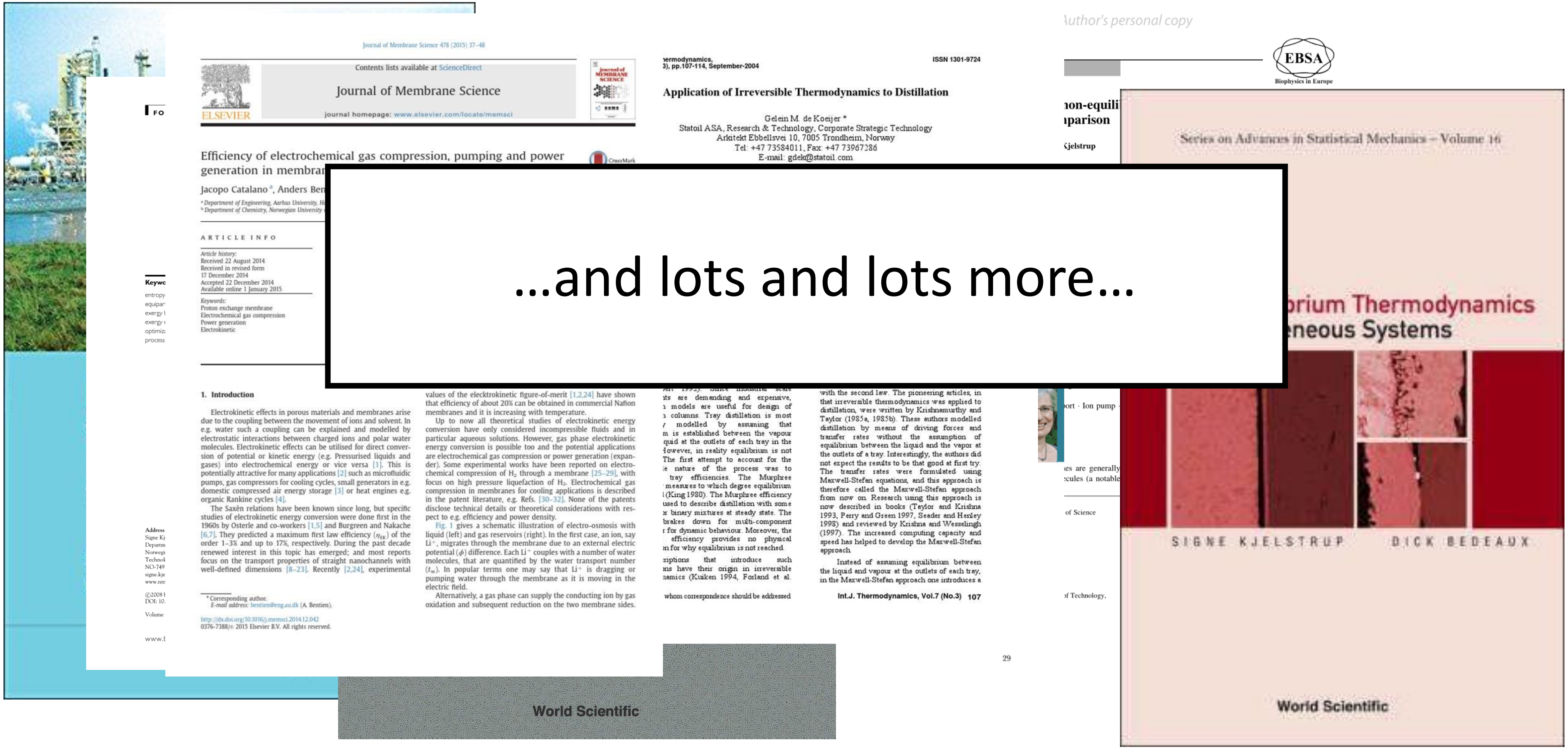
Efficiency of electrochemical gas compression, pumping and power generation in membranes
Jacopo Catalano, Anders Bentien, David Nicolas Østedgaard-Munck, Signe Kjelstrup
1. Introduction
Application of Irreversible Thermodynamics to Distillation
Gelein M. de Koeijer
Statoil ASA, Research & Technology, Corporate Strategic Technology
Signe Kjelstrup
Norwegian University of Science and Technology, Department of Chemistry
Int.J. Thermodynamics, Vol.7 (No.3) 107
ISSN 1301-9724
World Scientific
Author's personal copy
EBSA
Biophysics in Europe
Series on Advances in Statistical Mechanics – Volume 16
Non-Equilibrium Thermodynamics of Heterogeneous Systems
SIGNE KJELSTRUP
DICK BEDEAUX
World Scientific

2010


Journal of Membrane Science
Efficiency of electrochemical gas compression, pumping and power generation in membran
Application of Irreversible Thermodynamics to Distillation
Series on Advances in Statistical Mechanics – Volume 16
SIGNE KJELSTRUP
DICK BEDEAUX
World Scientific
…and lots and lots more…

2013

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


Santanu Sinha
Isha Savani
Alex Hansen
Signe Kjelstrup
Morten Vassvik
Dick Bedeaux

2017

Dealing with thermodynamics

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

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

Three Laws of Thermodynamics

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

Thermodynamics: Two-Phase Flow

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

CrossMark

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

Isha Savani[1] · Santanu Sinha[2] · Alex Hansen[2] ·
Dick Bedeaux[3] · Signe Kjelstrup[3] · Morten Vassvik[1]

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

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

Signe Kjelstrup [1], Dick Bedeaux [1], Alex Hansen [2], Bjørn Hafskjold [1] and Olav Galteland [1]*

[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)

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

Signe Kjelstrup [1], Dick Bedeaux [1], Alex Hansen [2], Bjørn Hafskjold [1] and Olav Galteland [1]*

[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)

«Thermodynamics»

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

Alex Hansen[1] · Santanu Sinha[2] · Dick Bedeaux[3] · Signe Kjelstrup[3] · Magnus Aa. Gjennestad[1] · Morten Vassvik[1]

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

«Thermodynamics»

Core idea of thermodynamics:
Euler homogeneous functions and energy conservation

«Thermodynamics»

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

«Thermodynamics»

Mass conservation

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

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

«Thermodynamics»

Mass conservation

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

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

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

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

«Thermodynamics»

Mass conservation

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

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

«Thermodynamics»

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

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

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

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«Thermodynamics»

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

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

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

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

Constitutive Equations

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

Constitutive Equations

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

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

Constitutive Equations

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

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

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

Constitutive Equations

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

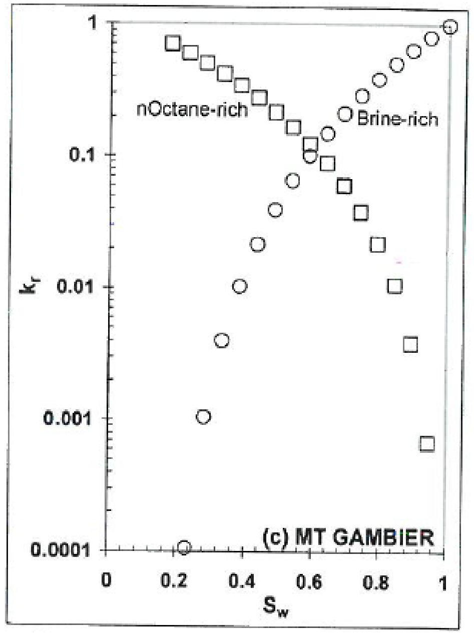
Constitutive Equations

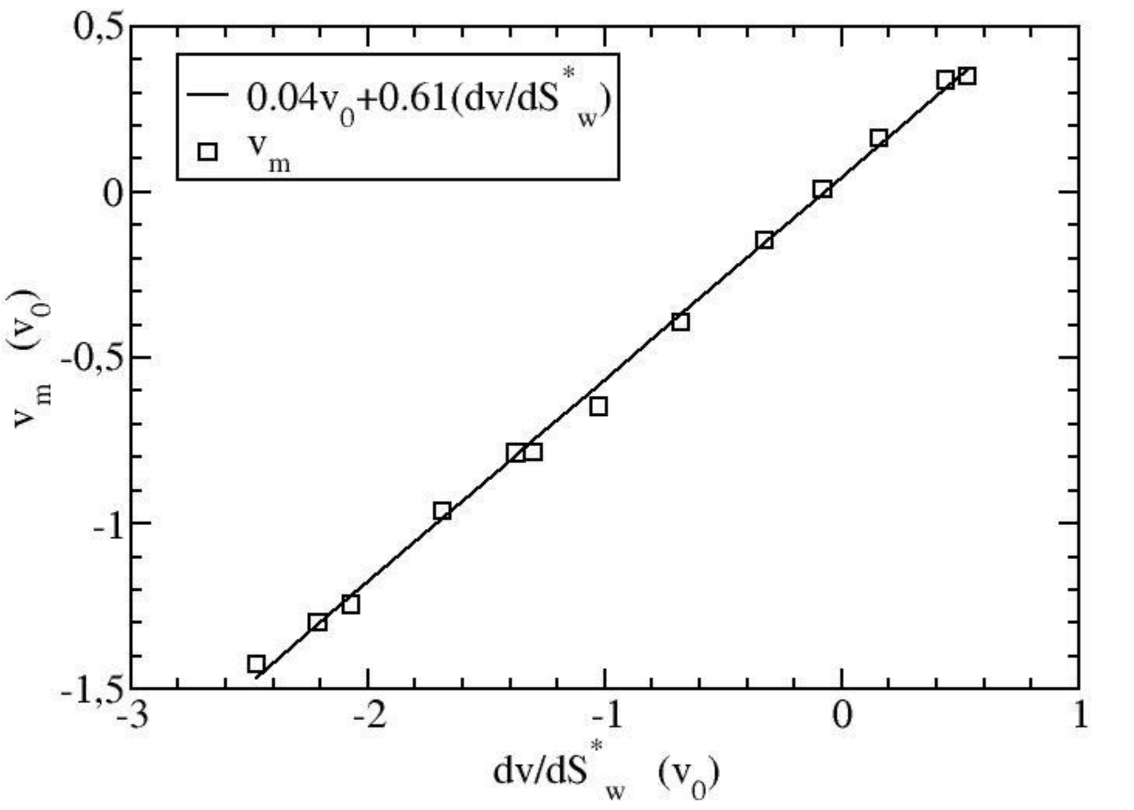
SPE 113386

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

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.





Constitutive Equations

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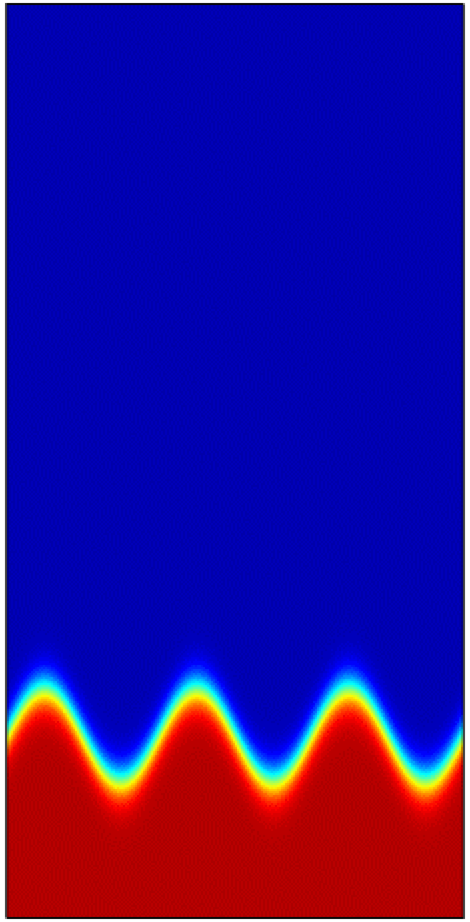
$$\mathbf{v}_m = -\tilde{B}\nabla(P - P_c) + \tilde{M}\frac{d^2 P_c}{dS_w^2}\nabla S_w$$

Where relative permeability is ok.

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

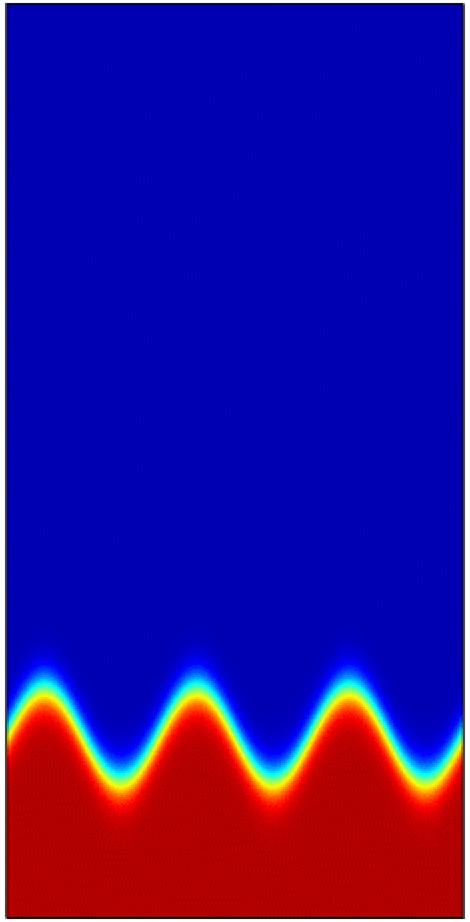
Immiscible Two-Phase Flow

Imbibition



Immiscible Two-Phase Flow

Imbibition

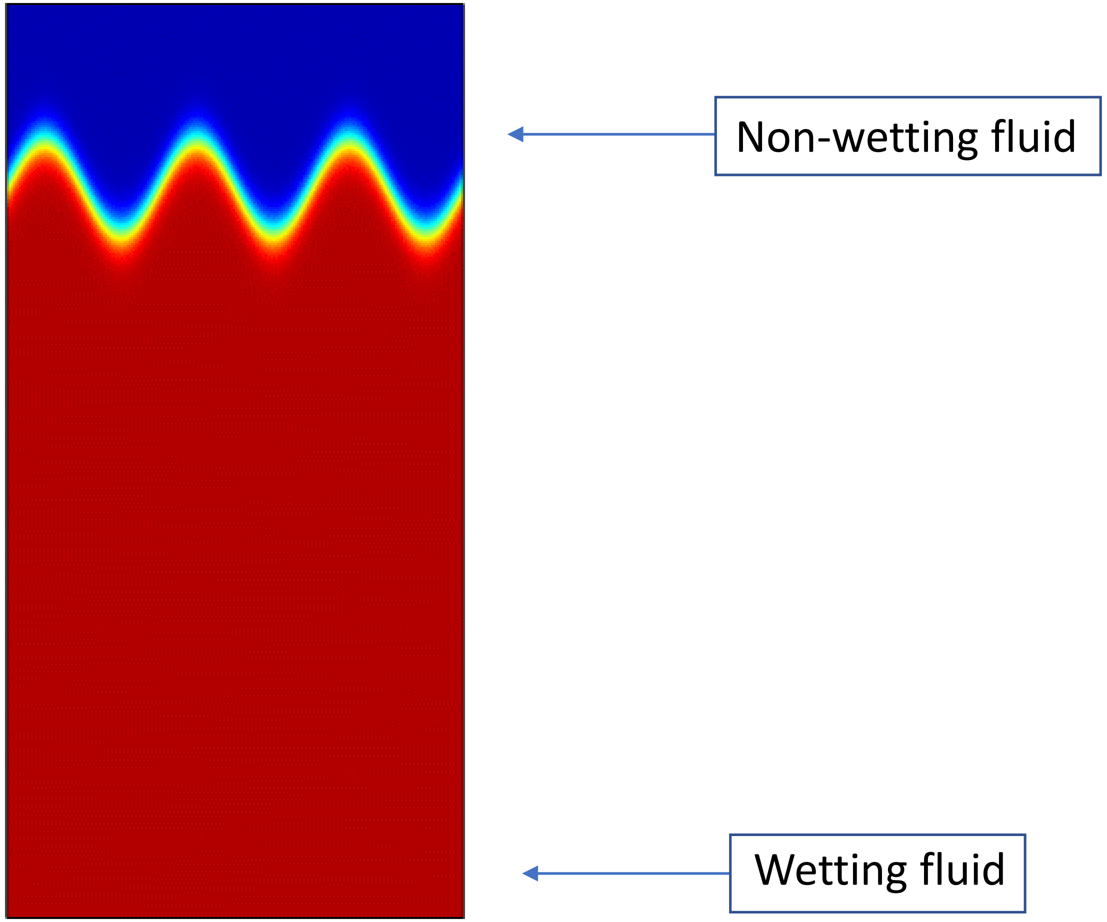


Non-wetting fluid

Wetting fluid

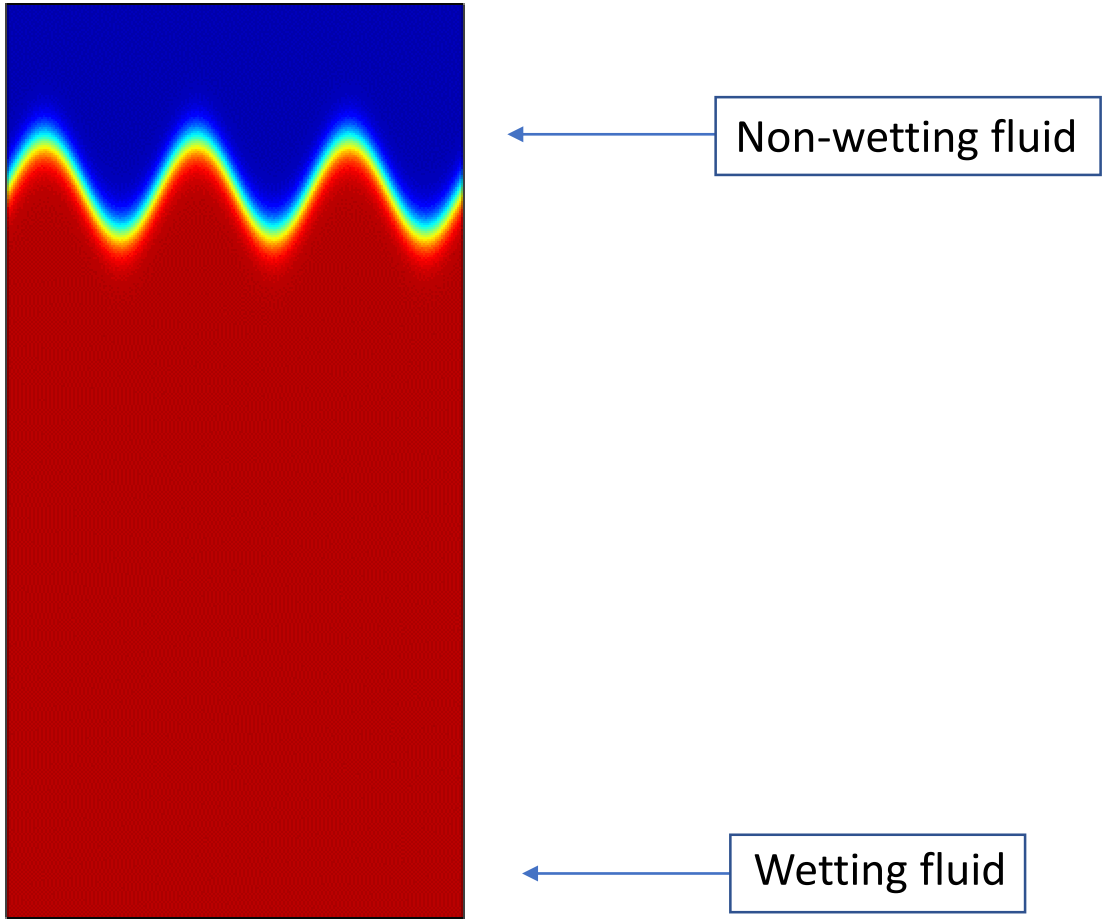
Immiscible Two-Phase Flow

Drainage



Immiscible Two-Phase Flow

Drainage



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