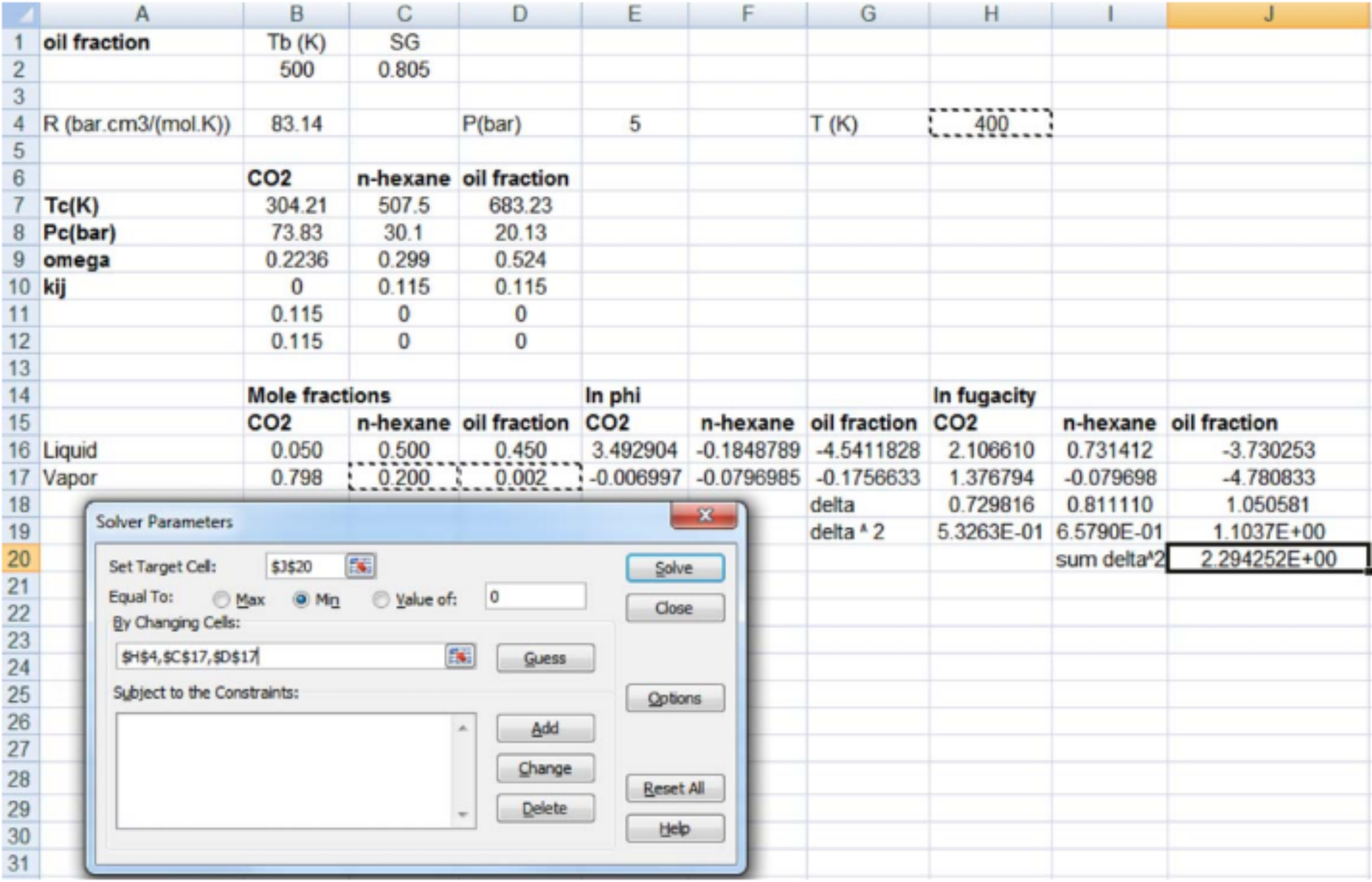
European Symposium on Applied Thermodynamics
May 18-21, 2017, Bucharest, Romania

XSEOS
Thermodynamic Properties using Excess Gibbs Free Energy Models and Equations of State

	Excess Gibbs free energy	Equations of state
Models	Margules 2-,3-,4-suffix	van der Waals
	Regular solution theory	Redlich-Kwong
	Flory-Huggins	Soave-Redlich-Kwong (SRK)
	Wilson	Peng-Robinson (PR)
	TK-Wilson	PR, quadratic mixing rule for b
	NRTL	Stryjek-Vera
	UNIQUAC	Predictive SRK (PSRK)
	UNIFAC	Mattedi-Tavares-Castier (MTC)
	Modified UNIFAC (Dortmund)	

https://people.qatar.tamu.edu/marcelo.castier/index.htm

	A	B	C	D	E	F	G	H	I	J
1	**oil fraction**	Tb (K)	SG							
2		500	0.805							
3										
4	R (bar.cm3/(mol.K))	83.14		P(bar)	5		T (K)	400		
5										
6		**CO2**	**n-hexane**	**oil fraction**						
7	**Tc(K)**	304.21	507.5							
8	**Pc(bar)**	73.83	30.1							
9	**omega**	0.2236	0.299							
10	**kij**	0	0.115	0.115						
11		0.115	0	0						
12		0.115	0	0						
13										
14		**Mole fractions**			**ln phi**			**ln fugacity**		
15		**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**
16	Liquid	0.050	0.500	0.450						
17	Vapor	0.798	0.200	0.002						
18							delta			
19							delta ^ 2			
20									sum delta^2	



	A	B	C	D	E	F	G	H	I	J
1	**oil fraction**	Tb (K)	SG							
2		500	0.805							
3										
4	R (bar.cm3/(mol.K))	83.14		P(bar)	5		T (K)	400		
5										
6		**CO2**	**n-hexane**	**oil fraction**						
7	**Tc(K)**	304.21	507.5	683.23						
8	**Pc(bar)**	73.83	30.1	20.13						
9	**omega**	0.2236	0.299	0.524						
10	**kij**	0	0.115	0.115						
11		0.115	0	0						
12		0.115	0	0						
13										
14		**Mole fractions**			**ln phi**			**ln fugacity**		
15		**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**
16	Liquid	0.050	0.500	0.450	3.492904	-0.1848789	-4.5411828	2.106610	0.731412	-3.730253
17	Vapor	0.798	0.200	0.002	-0.006997	-0.0796985	-0.1756633	1.376794	-0.079698	-4.780833
18							delta	0.729816	0.811110	1.050581
19							delta ^ 2	5.3263E-01	6.5790E-01	1.1037E+00
20									sum delta^2	2.294252E+00

	A	B	C	D	E	F	G	H	I	J
1	**oil fraction**	Tb (K)	SG							
2		500	0.805							
3										
4	R (bar.cm3/(mol.K))	83.14		P(bar)	5		T (K)	318.268697		
5										
6		**CO2**	**n-hexane**	**oil fraction**						
7	**Tc(K)**	304.21	507.5	683.23						
8	**Pc(bar)**	73.83	30.1	20.13						
9	**omega**	0.2236	0.299	0.524						
10	**kij**	0	0.115	0.115						
11		0.115	0	0						
12		0.115	0	0						
13										
14		**Mole fractions**			**ln phi**			**ln fugacity**		
15		**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**	**CO2**	**n-hexane**	**oil fraction**
16	Liquid	0.050	0.500	0.450	2.920869	-2.394525	-8.7905024	1.534575	-1.478234	-7.979572
17	Vapor	0.949	0.051	8.82E-05	-0.022062	-0.1180327	-0.2527156	1.534595	-1.478200	-7.979583
18							delta	-0.000020	-0.000034	0.000011
19							delta ^ 2	4.1184E-10	1.1570E-09	1.1473E-10
20									sum delta^2	1.683616E-09

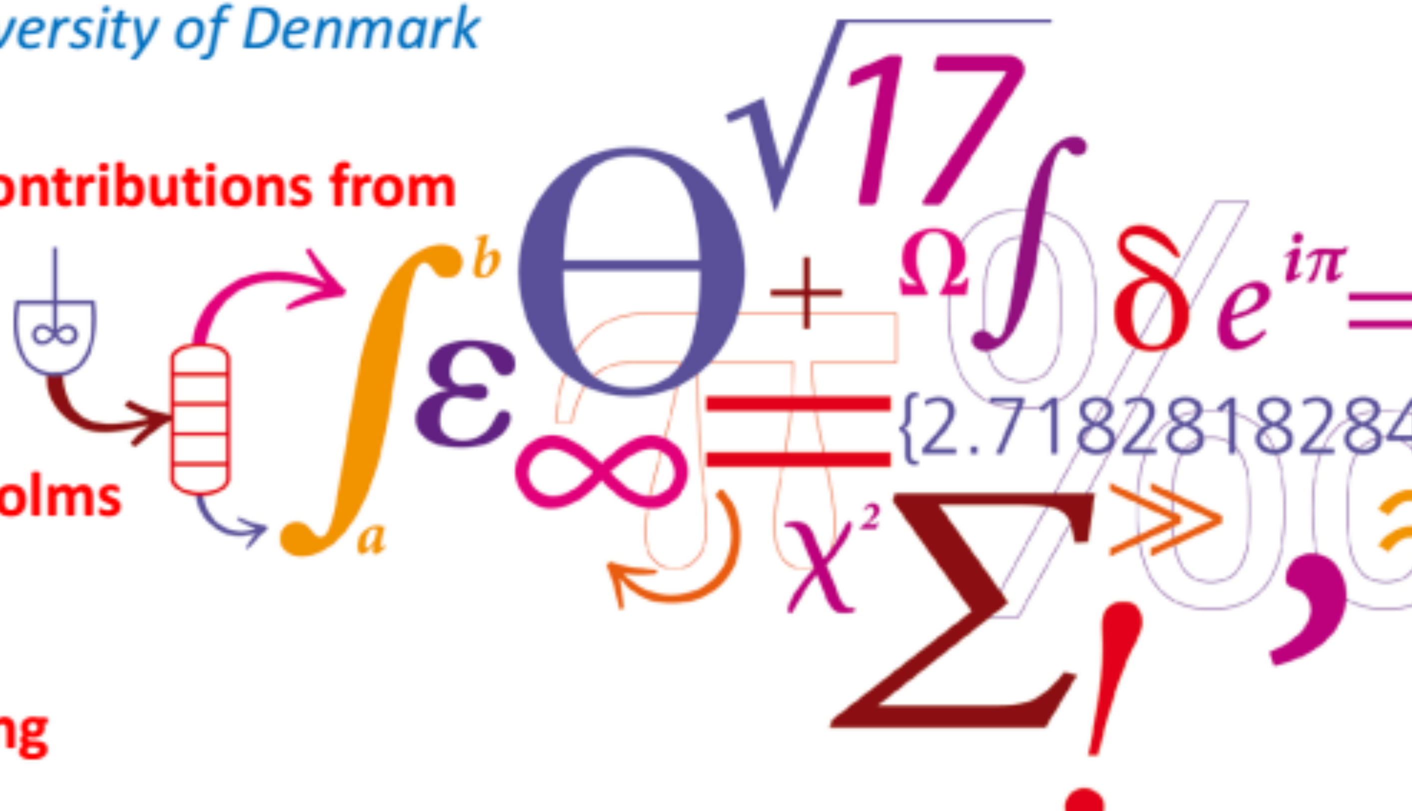
Teaching Chemical Engineering Thermodynamics at DTU

How, Why, Impressions, Some Personal Thoughts

Georgios M. Kontogeorgis
Center for Energy Resources Engineering (CERE)
Department of Chemical and Biochemical Engineering
Technical University of Denmark

With great contributions from All "Thermo" Teachers:

Nicolas von Solms
Kaj Thomsen
Wei Yan
Xiaodong Liang



Teaching Thermodynamics – Content

Course Number	Name	Content
28221 28322	Chemical Eng. Thermodynamics	Pure compounds, mixtures, cycles, flash calculations, process applications e.g. refrigeration, ternary LLE, acivity coefficient models
28423	Phase Equilibria for non-ideal mixtures	Cubic and non-cubic EoS (SAFT, CPA), mixing rules for cubic EoS, polymers, environmental thermodynamics, electrolytes
28909	Thermodynamic models: Fundamentals and Computational aspects	Computational methods : PT flash, Multiphase flash, stability analysis, chemical equilibrium
28928	Electrolyte Thermodynamics	Electrolytes fundamentals, phase diagrams and models
28917	Statistical Thermodynamics	Fundamentals, CS EoS, Monte Carlo simulations, SAFT

Teaching Thermodynamics – Special Issues

Course Number	Name	Special Issues	Comments
28221 28322	Chemical Eng. Thermodynamics	Use of excel modules No written examination – only reports	Own teaching material + one other book
28423	Phase Equilibria for non-ideal mixtures	Use of SPECS	Own teaching material
28909	Thermodynamic models: Fundamentals and Computational aspects	Own coding (Fortran, MATLAB), many externals incl. Industrial participants	Own teaching material
28928	Electrolyte Thermodynamics	On-line course	Own teaching material
28917	Statistical Thermodynamics	Sometimes student-defined projects	Book from literature

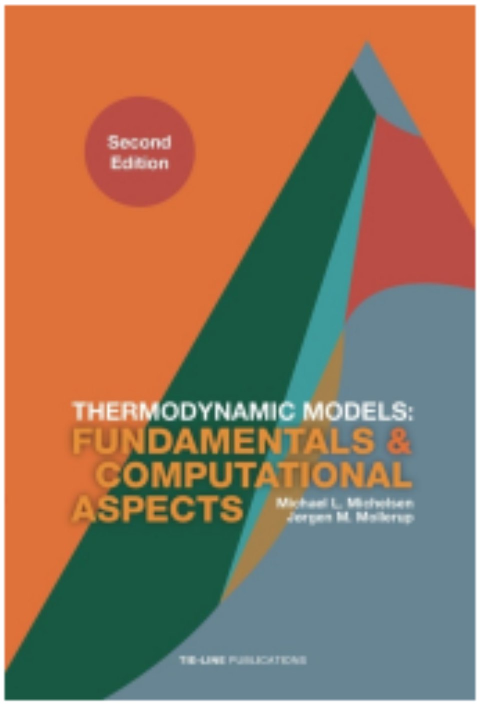
Teaching Thermodynamics – Book

Course Number	Name	Book
28221 28322	Chemical Eng. Thermodynamics	Elliott & Lira + Michelsen Notes
28423	Phase Equilibria for non-ideal mixtures	Kontogeorgis & Folas K. Thomsen Notes
28909	Thermodynamic models: Fundamentals and Computational aspects	Michelsen & Mollerup
28928	Electrolyte Thermodynamics	K. Thomsen Notes
28917	Statistical Thermodynamics	McQuarrie

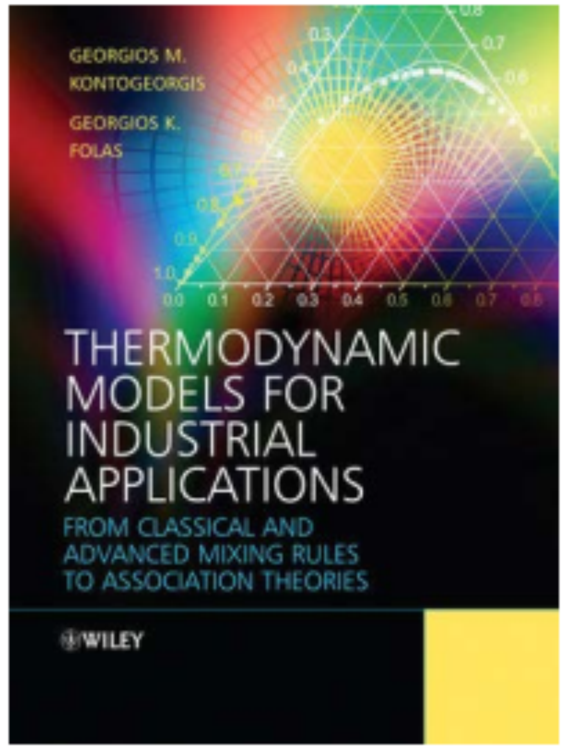
Books in Thermodynamics (by CERE staff)

Mostly used in the PhD Course:

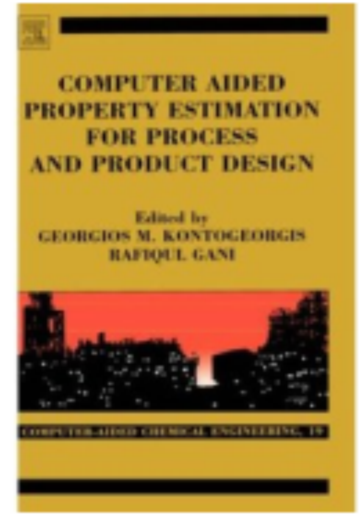
28909 (2007)

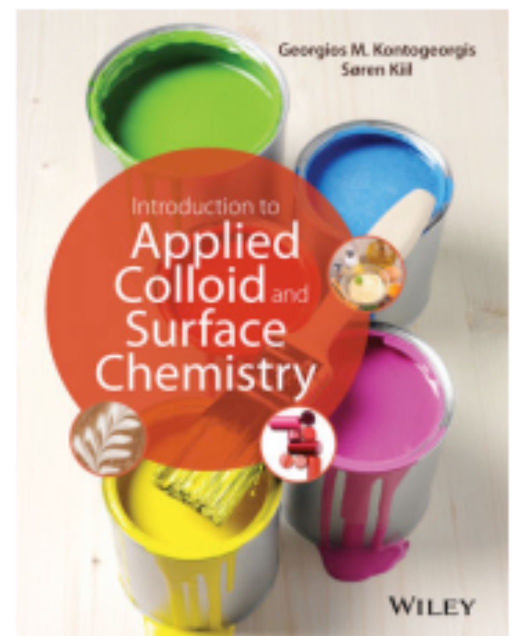


28423 (2010)



(2004)





Kaj Thomsen : Notes on Electrolyte Thermodynamics (very extensive) +
special course with exercises

M.L.Michelsen : Notes on Applied Thermodynamics with exercises

DTU vs. Rest of the world (survey) – The Books

- We use Elliott and Lira like 14 US and none European universities – in one of the courses
- We do not use Sandler and have abandoned long time ago the most popular Smith-van Ness-Abbott book
- We recommend Prausnitz el al. in our advanced courses
- Atkins is used in Physical Chemistry courses – not in thermodynamics
- We have lots of own books/own book material

DTU vs. Rest of the world (survey)

- We have also ”the two basic” courses – but also a PhD course on computational aspects
- We have more additional specialized thermodynamic courses
- Not much on biological systems (similar to Europe)
- SM and MS – to limited degree but we have them
- Similarly to others, no experimental element in the courses (despite much experimental thermodynamics in research)
- More PBL in USA than in Europe – we also are based much on PBL