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First Principles Compaction, Phase Equilibrium, & Kinetics

Basin Modeling Context

Dr. Annette Fugl

Introduction

name: Annette Fugl

education: MSc ME - fluid/solid mechanics
PhD - circulation fluidized bed
OJT - basin modeling
Post Doc - 3D basin modeling

experience: Development of basin models

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Agenda

- First principles
  - Compaction
  - Phase equilibrium
  - Organic kinetics
- Outline
  - Backgound
  - Method
  - Basin modeling context
- Issues
- Conclusion

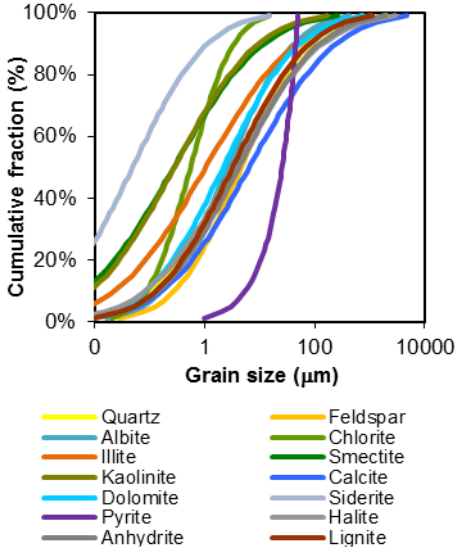
Compaction - Background

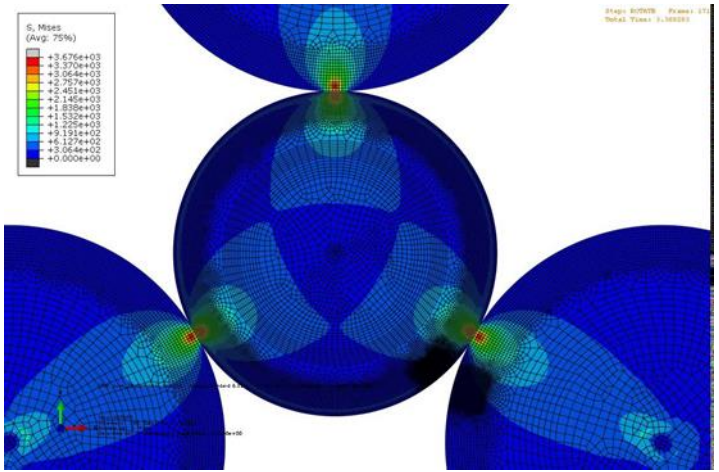
- Terzaghi's principle
  - Constant volume compressibility
  - Relationship between void ratio and effective stress independent of time
  - Compression one-dimensional
  - Empirical volume compressibility

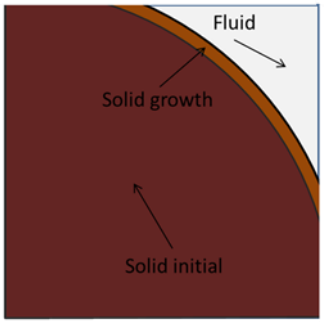
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Compaction - Geometry

- Contact interfacial area
- Ellipsoid grain with log-normal size distribution



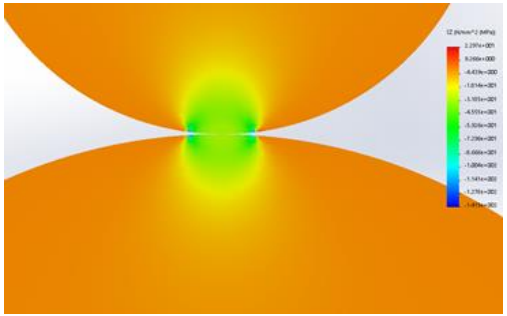




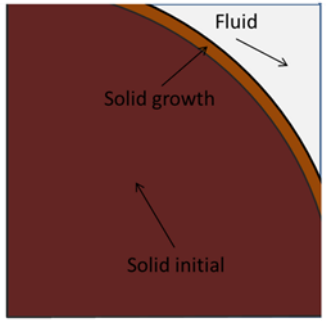
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Compaction - Dynamics

- Redistribution of mineral atoms near contact area
- Diffusion of elastic strain
- Creeping flow tied to Stokes law & effective stress

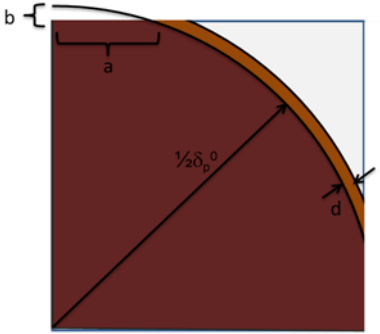


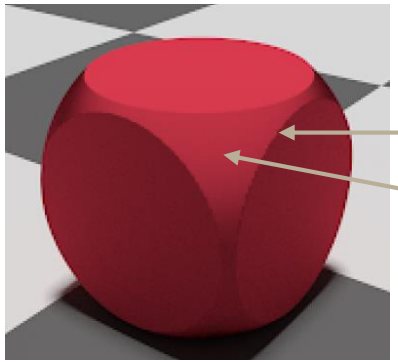
$$u = \frac{d\delta_p}{dt} = \frac{1}{2\mu} R_H^2 \frac{\sigma_r - p}{\Delta L}$$



Compaction - Dynamics

- Drag coefficient tied to Reynolds number & hydraulic radius





$$\left.\begin{aligned} R_H &= \frac{A_{SF}}{p_{SF}} \\ p_{SF} &= 12\,\pi\,a \\ A_{SF} &= \pi\left(\delta_p\right)^2 - 3\pi\delta_p(b+d) \\ a^2 &= \left(\frac{\delta_p^0}{2}+d\right)^2 - \left(\frac{\delta_p^0}{2}-b\right)^2 \end{aligned}\right\} \Rightarrow R_H = \frac{\left(\delta_p\right)^2 - 3\delta_p\left(b+\frac{\delta_p-\delta_p^0}{2}\right)}{12\sqrt{\left(\frac{\delta_p}{2}\right)^2 - \left(\frac{\delta_p^0}{2}-b\right)^2}}$$

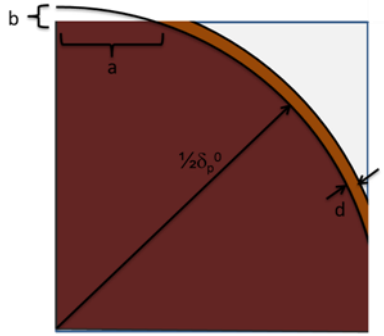
Compaction - Dynamics

- Geometrical constraint
  - Thickness of the solid under strain is assumed to be the indent in the original grain, b
  - Constant solid volume
  - Porosity tied to packing

$$\Delta L = b$$

$$V_{identation} = V_{growth}$$

$$1 - \phi = \frac{\pi}{6} \frac{1}{\left(1 - 2\,b/\delta_p^0\right)^3}$$

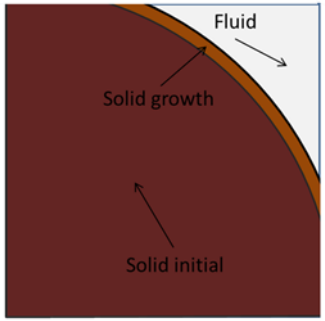


- Rock stress & over burden

$$\sigma_{ob} = (1 - \phi)\,\sigma_r + \phi\,p$$

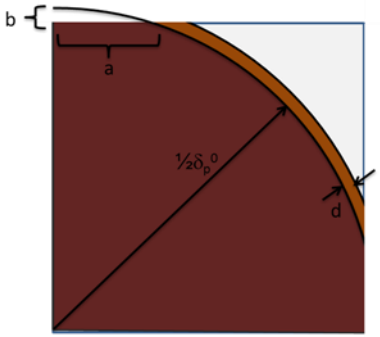
$$\sigma_r = \frac{\sigma_{ob} - \phi\,p}{1 - \phi}$$

$$\sigma_r - p = \frac{\sigma_{ob} - \phi\,p - p + \phi\,p}{1 - \phi} = \frac{\sigma_{ob} - p}{1 - \phi}$$



Compaction - Dynamics

- Ordinary differential equation for grain size evolution



$$\frac{d\delta_p}{dt} = \frac{\sigma_e}{\mu}\frac{6\left(\delta_p^0 - 2b\right)^3}{\pi\left(\delta_p^0\right)^3} f\left(\delta_p, b\right) = \frac{\sigma_e}{\mu} f_{HR}\left(\delta_p, b\right)$$

$$f_{HR}\left(\delta_p, b\right) = \frac{\left(\delta_p^0 - 2b\right)^3 \left(\left(\delta_p\right)^2 - 3\delta_p\left(b + \frac{\delta_p - \delta_p^0}{2}\right)\right)^2}{12\pi\left(\delta_p^0\right)^3 b\left(\left(\delta_p\right)^2 - \left(\delta_p^0 - 2b\right)^2\right)}$$

Compaction - Data

- Viscosity tied to shear modulus, dislocation frequency & temperature
- Arrhenius type dislocation frequency
- Activation energy from Wood's compensation law

$$\mu = G\,\tau$$

$$G = \frac{E}{2(1+\nu)}$$

$$\tau = \frac{1}{k}$$

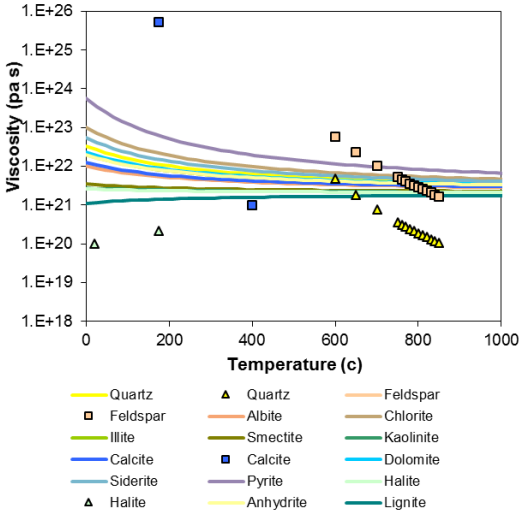
$$k = A\,exp\left(\frac{-E_A}{RT}\right)$$

$$E_A = 5505\,log\left(\frac{A}{A_{ref}}\right)$$

$$A = G/\mu_{ref}$$

$$A_{ref} = G_{ref}/\mu_{ref}$$

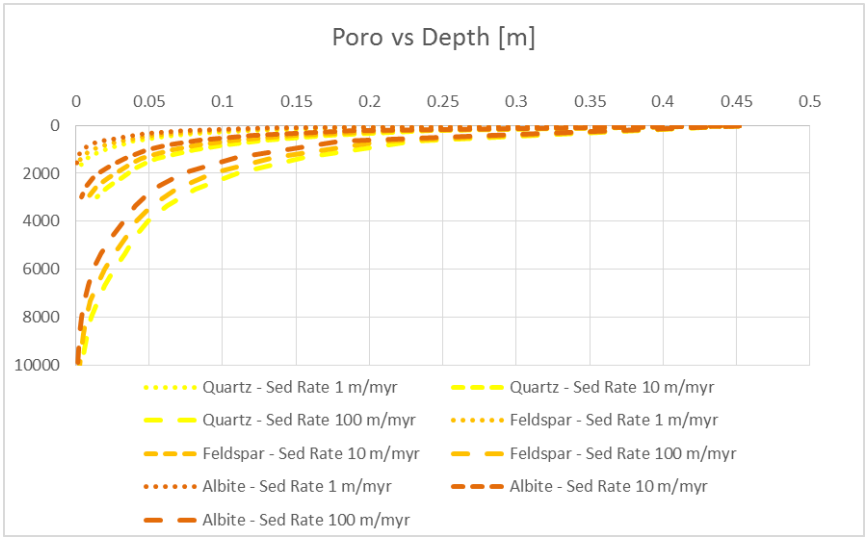
$$\mu = \mu_{ref}\left(\frac{G}{G_{ref}}\right)^{\frac{5505}{RT}}$$

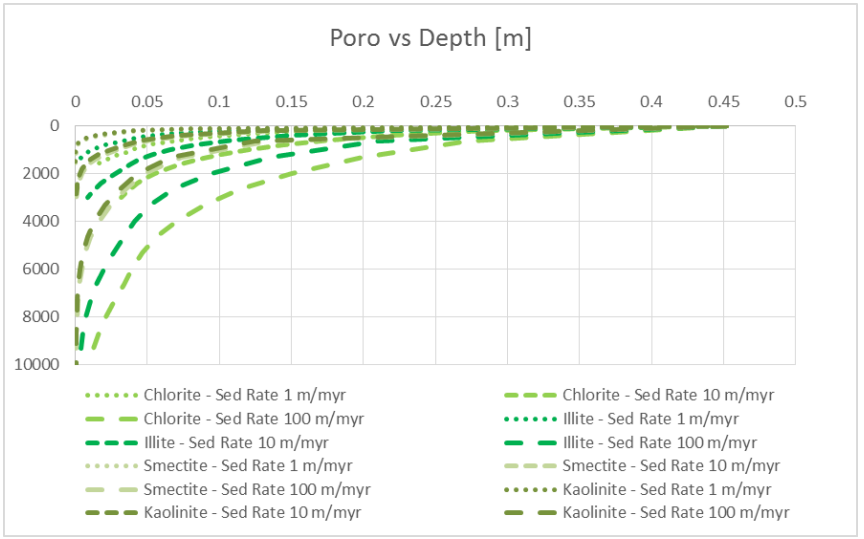


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Compaction - Data

- Porosity versus depth for varying sedimentation rates

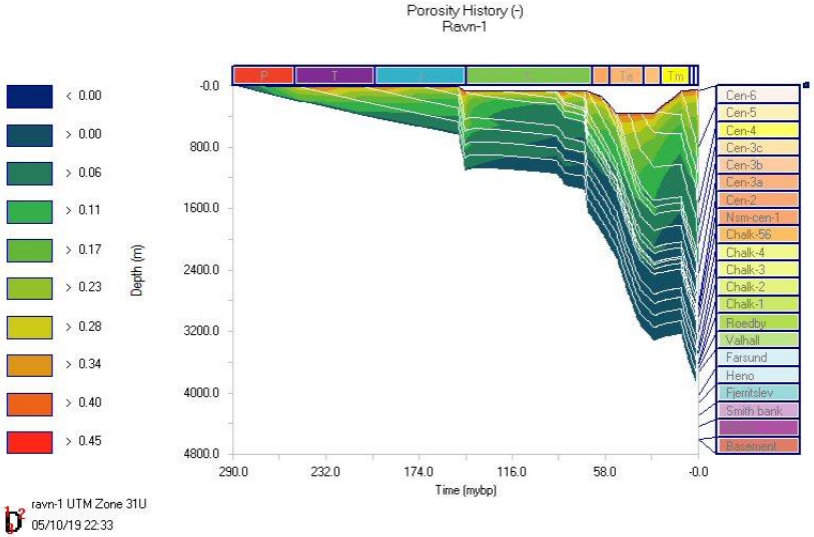


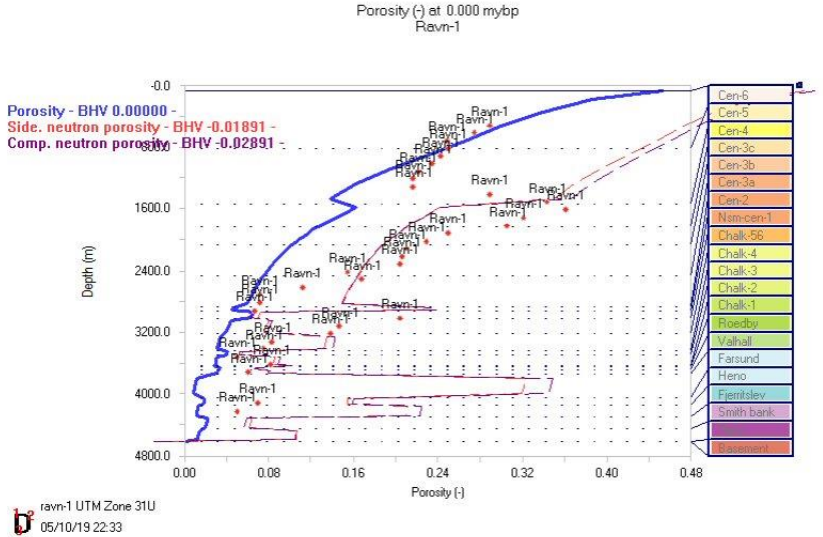


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Compaction – Basin Modeling

- Porosity Subsidence profile
- Porosity - Depth profile





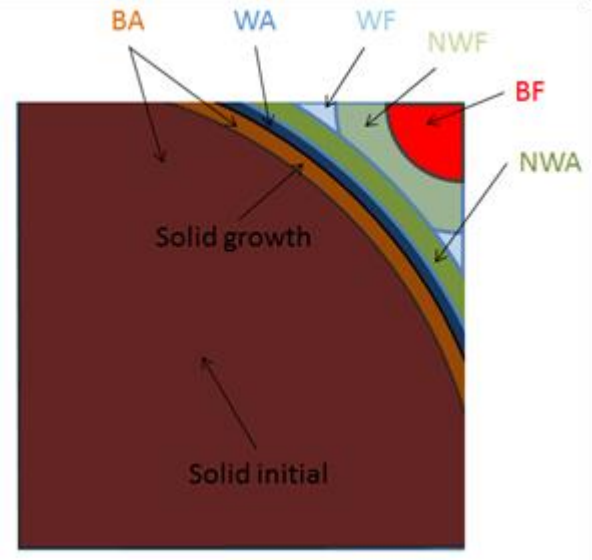
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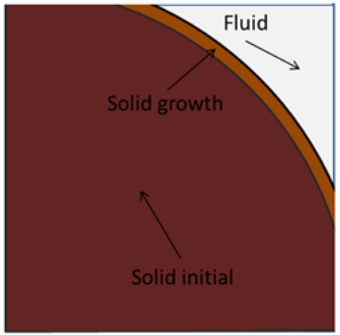
Phase Equilibrium - Background

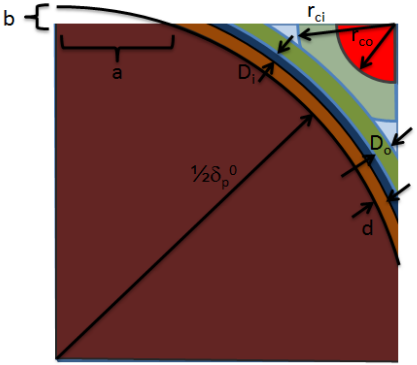
- Empirical data
  - Capillary pressure-saturation curves
  - Critical/Connate saturation
  - Adsorption (Freundlich/Langmuir)
  - Equation of State (Peng-Robinson)
- Multi-component phase distribution (two phases)
- Compositional grading

Phase Equilibrium - Geometry

- Cap-deformed ellipsoid solid phase
- 2 adsorbed film & 3 free fluid phases







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Phase Equilibrium - Dynamics

- Phase internal & external molecular interaction
- Interaction potential tied to polarizability, dipole moment, & charge

Interaction - structural elements

Fixed dipole



Freely rotating dipole

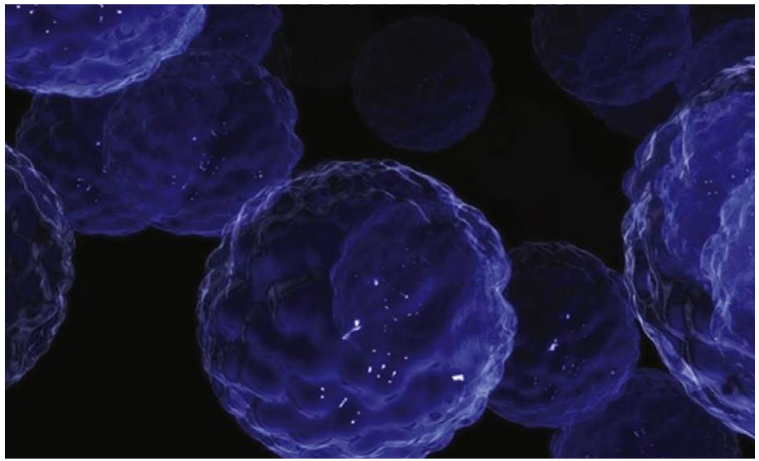


Induced dipole



Electric charge (ion)





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Molar Specific Energy & Interaction Potential

- Interaction between induced dipoles of molecule *i* & *l*

$$\varphi_{33}^{il} = \frac{-3}{2r^6}\,\frac{1}{(4\pi\varepsilon_0)^2}\,\alpha_i\alpha_l h\frac{f_i f_l}{f_i + f_l} \qquad g_{i,33}^{jk} = \sum_l \int_{V_{min}^{ii}}^{\infty} N_l \varphi_{33}^{il} dV = \sum_l \frac{-h\alpha_i\alpha_l}{8\pi\varepsilon_0^2\left(\delta_{jk}^i\right)^3}\frac{f_i f_l}{f_i + f_l} N_l$$

$$\varphi_{N33}^{il} = \frac{-V_{ci}V_{cl}}{(N_A)^2\frac{2}{3}r^6}\frac{\lambda_{Ni}\lambda_{Nl}T_{cl}}{(\lambda_{Ni}T_{ci} + \lambda_{Nl}T_{cl})}\alpha_{Ni}\alpha_{Nl} \qquad \int_{V_{min}^{jk}}^{V^{jk}} \frac{1}{r^6} dV = \int_{\delta_{jk}^i}^{\infty} 4\pi\frac{r^2}{r^6} dr = \frac{4\pi}{3\left(\delta_{jk}^i\right)^3}$$

$$g_{Ni,33}^{jk} = \sum_l \frac{-V_{ci}V_{cl}2\pi}{(N_A)^2\left(\delta_{jk}^i\right)^3}\frac{\lambda_{Ni}\lambda_{Nl}T_{cl}}{(\lambda_{Ni}T_{ci} + \lambda_{Nl}T_{cl})}\alpha_{Ni}\alpha_{Nl}N_l$$

Phase Equilibrium – Interaction Potential I

p q	Interaction potential term	$-G^{j,m}_{Nil,pq}/A_{j,m}$		$-\frac{\partial G^{j,m}_{Nil,pq}}{\partial n^{j}_{i}}/A_{j,m}$		$-g^{j}_{Ni,pq}$	
	[kT_{ci} – J/molecule]	[N/m]		[Jm/mol]		[J/mol]	
11	$\sqrt{V_{ci}V_{cl}}\sqrt{\frac{T_{cl}}{T_{ci}}}\sqrt{\delta_{Ni}\delta_{Nl}}\left(2\cos(\Theta_i)\cos(\Theta_l)-\sin(\Theta_i)\sin(\Theta_l)\cos(\varphi_{il})\right)$	$\frac{3}{8\pi}N_A^{2/3}$	$n_i^{5/3}$	$\frac{5}{8\pi}N_A^{2/3}$	$n_i^{2/3}$	$\frac{3}{8\pi}N_A$	n_i
13	$V_{ci}V_{cl}\delta_{Ni}\alpha_{Nl}\left(1+3\cos^2(\Theta_i)\right)$	$\frac{1}{32\delta_{jk}^2}=\frac{\pi}{8B_a}$	$n_i n_l$	$\frac{1}{32\delta_{jk}^2}=\frac{\pi}{8B_a}$	n_l	$\frac{1}{2\delta_{jk}^3}=\frac{2\pi N_A}{3B_V}$	n_l
14	$\sqrt{V_{ci}}(V_{cl})^{\frac{1}{6}}\sqrt{\frac{T_{cl}}{T_{ci}}}\sqrt{\delta_{\mathrm{Ni}}}\tau_{\mathrm{Nl}}\cos(\Theta_i)$	$\frac{\sqrt{3}}{8\pi}N_A^{2/3}$	$n_i^{4/3}$	$\frac{1}{2\sqrt{3}\pi}N_A^{2/3}$	$n_i^{1/3}$	0	-
22	$V_{ci}V_{cl}\frac{T_{cl}}{T}\delta_{Ni}\delta_{Nl}$	$\frac{1}{64\pi\delta_{jk}^2}=\frac{1}{16B_a}$	$n_i n_l$	$\frac{1}{64\pi\delta_{jk}^2}=\frac{1}{16B_a}$	n_l	$\frac{1}{4\pi\delta_{jk}^3}=\frac{N_A}{3B_V}$	n_l
23	$V_{ci}V_{cl}\alpha_{Nl}\delta_{Ni}$	$\frac{1}{16\delta_{jk}^2}=\frac{\pi}{4B_a}$	$n_i n_l$	$\frac{1}{16\delta_{jk}^2}=\frac{\pi}{4B_a}$	n_l	$\frac{1}{\delta_{jk}^3}=\frac{4\pi N_A}{3B_V}$	n_l
24	$V_{ci}(V_{cl})^{\frac{1}{3}}\frac{T_{cl}}{\mathrm{T}}\delta_{Ni}(\tau_{Nl})^2$	$\frac{1}{64\pi^2}N_A^{2/3}$	n_i^2	$\frac{1}{32\pi^2}N_A^{2/3}$	n_i	$\frac{N_A^{2/3}}{8\pi\delta_{jk}}=\frac{N_A}{\sqrt[3]{384\pi^2 B_V}}$	n_l
31	$V_{ci}V_{cl}\delta_{Nl}\alpha_{Ni}\left(1+3\cos^2(\Theta_l)\right)\frac{T_{cl}}{T_{ci}}$	$\frac{1}{32\delta_{jk}^2}=\frac{\pi}{8B_a}$	$n_i n_l$	$\frac{1}{32\delta_{jk}^2}=\frac{\pi}{8B_a}$	n_l	$\frac{1}{2\delta_{jk}^3}=\frac{2\pi N_A}{3B_V}$	n_l
32	$V_{ci}V_{cl}\alpha_{Ni}\delta_{Nl}\frac{T_{cl}}{T_{ci}}$	$\frac{1}{16\delta_{jk}^2}=\frac{\pi}{4B_a}$	$n_i n_l$	$\frac{1}{16\delta_{jk}^2}=\frac{\pi}{4B_a}$	n_l	$\frac{1}{\delta_{jk}^3}=\frac{4\pi N_A}{3B_V}$	n_l

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Phase Equilibrium – Interaction Potential II

p q	Interaction potential term	$-G^{j,m}_{Nil,pq}/A_{j,m}$		$-\frac{\partial G^{j,m}_{Nil,pq}}{\partial n_i^j}/A_{j,m}$		$-g^{j}_{Ni,pq}$	
	[kT_{ci} – J/molecule]	[N/m]		[Jm/mol]		[J/mol]	
33	$V_{ci}V_{cl}\frac{\lambda_{Ni}\lambda_{Nl}T_{cl}}{(\lambda_{Ni}T_{ci}+\lambda_{Nl}T_{cl})}\alpha_{Ni}\alpha_{Nl}$	$\frac{\pi}{8\delta_{jk}^2}=\frac{\pi^2}{2B_a}$	$n_i n_l$	$\frac{\pi}{8\delta_{jk}^2}=\frac{\pi^2}{2B_a}$	n_l	$\frac{2\pi}{\delta_{jk}^3}=\frac{8\pi^2 N_A}{3B_V}$	n_l
34	$V_{ci}(V_{cl})^{\frac{1}{3}}\alpha_{Ni}(\tau_{Nl})^2\frac{T_{cl}}{T_{ci}}$	$\frac{1}{16\pi}N_A^{2/3}$	n_i^2	$\frac{1}{8\pi}N_A^{2/3}$	n_i	$\frac{1}{2\delta_{jk}}N_A^{2/3}=\sqrt[3]{\frac{\pi}{6}}\frac{N_A}{\sqrt[3]{B_V}}$	n_l
41	$\sqrt{V_{cl}}(V_{ci})^{\frac{1}{6}}\sqrt{\frac{T_{cl}}{T_{ci}}}\sqrt{\delta_{Nl}}\tau_{Ni}\cos(\theta_l)$	$\frac{\sqrt{3}}{8\pi}N_A^{2/3}$	$n_i^{4/3}$	$\frac{1}{2\sqrt{3}\pi}N_A^{2/3}$	$n_i^{1/3}$	0	-
42	$V_{cl}(V_{ci})^{\frac{1}{3}}\frac{T_{cl}}{T}\delta_{Nl}(\tau_{Ni})^2$	$\frac{1}{64\pi^2}N_A^{2/3}$	n_i^2	$\frac{1}{32\pi^2}N_A^{2/3}$	n_i	$\frac{1}{8\pi\delta_{jk}}N_A^{2/3}=\frac{N_A}{\sqrt[3]{384\pi^2 B_V}}$	n_l
43	$V_{cl}(V_{ci})^{\frac{1}{3}}\alpha_{Nl}(\tau_{Ni})^2$	$\frac{1}{16\pi}N_A^{2/3}$	n_i^2	$\frac{1}{8\pi}N_A^{2/3}$	n_i	$\frac{1}{2\delta_{jk}}N_A^{2/3}=\sqrt[3]{\frac{\pi}{6}}\frac{N_A}{\sqrt[3]{B_V}}$	n_l
44	$(V_{ci})^{\frac{1}{6}}(V_{cl})^{\frac{1}{6}}\sqrt{\frac{T_{cl}}{T_{ci}}}\tau_{Ni}\tau_{Nl}$	$\frac{-1}{8\pi}N_A^{2/3}$	n_i	$\frac{-1}{8\pi}N_A^{2/3}$	1	$\frac{-1}{8\pi}N_A$	n_i^1
55	$\sqrt{V_{ci}V_{cl}}\sqrt{\frac{T_{cl}}{T_{ci}}}\sqrt{\delta_{Ni}\delta_{Nl}}$	$\frac{3}{4\pi}N_A^{2/3}$	$n_i^{5/3}$	$\frac{5}{4\pi}N_A^{2/3}$	$n_i^{2/3}$	$\frac{3}{8\pi}N_A$	n_i
66	$\frac{T}{T_{ci}}exp\left(-\frac{1}{\kappa_{Ni}}\left(\frac{N_i V_{ci}}{N_A}\right)^{-1/3}\right)$	$36N_A^{2/3}$	$n_i^{2/3}$	$12N_A^{2/3}$	g_{66-A}	$288\pi N_A$	g_{6}

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Pressure & Molar Specific Energy

$$g = \sum_i x_i^j g_i + kT\, log\left(\frac{\rho}{1 - B\rho}\right) + \sum x_i F_i$$

$$p = \int_0^{\rho} \rho \frac{\partial \mathrm{g}}{\partial \rho}_T \, d\rho = \int_0^{\rho} \rho \frac{\partial}{\partial \rho} \sum\nolimits_i \left(x_i^j g_i\right)_T d\rho - \frac{kT}{B}\, log(1 - B\rho)$$

$$p = \sum\nolimits_i RT_{ci} x_i^{jk} \sum\nolimits_l \sum\nolimits_p \sum\nolimits_q \frac{n+m}{n+m+1} x_i^n x_l^m \rho^{n+m+1} \frac{gt_{Nil}^{pq} gc_{Nil}^{pq}}{\delta^k} - \frac{kT}{B}\, log(1 - B\rho)$$

$$B_j(T) = \frac{4\pi}{3}\delta^3 = 2b_{van\ der\ Waal} = \begin{cases} \sum_i x_{ij} B_{ij}(T) & mole\ arithmetic\ average\ of\ B_{ij} \\ \dfrac{\sum_i x_{ij} v_{ci}}{\sum_i \dfrac{x_i}{\omega_i(T)}} & critical\ volume\ hyperbolic\ average\ of\ B_{ij} \end{cases}$$

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PVT Single Phase – Single Component

$$\mathrm{p}\,(\rho) = -a^l\rho^2 - a^c\rho^{4/3} - \frac{RT}{B}\,log(1 - B\rho)$$

$$a^l = -\tfrac{1}{2}RT_c\left(\frac{gt_{Nil}^{22}gc_{Nil}^{22} + gt_{Nil}^{23}gc_{Nil}^{23} + gt_{Nil}^{32}gc_{Nil}^{32} + gt_{Nil}^{33}gc_{Nil}^{33}}{\delta^k}\right)$$

$$a^c = -\tfrac{1}{4}RT_c\,\frac{gt_{Nil}^{44}gc_{Nil}^{44}}{\delta^k}$$

$$\rho = \tfrac{1}{V}$$

$$p = -\frac{RT}{B}\,log(1 - B\rho) - \frac{a^l}{V^2} - \frac{a^c}{V^{4/3}} \approx \frac{RT}{V - B/2} - \frac{a}{V^2}$$

$$p = \frac{RT}{V - b} - \frac{a}{V^2} \qquad van\ der\ Waal$$

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PVT Single Phase – Single Component

$$T_r = \frac{T}{T_c} \qquad p_r = \frac{pV_c}{RT_c} \qquad \Omega(T_r) = \frac{B}{V_c}$$

$$v_r = \frac{V}{V_c} \qquad g_r = \frac{g}{RT_c} \qquad A(T_r) = \frac{f}{RT_cV_c}$$

$$a_r = \frac{a}{RT_c} \qquad s_r = \frac{s}{R} \qquad \Psi(T_r) = \frac{F}{RT_c} - T_r\, ln(V_c)$$

$$p_r = \frac{A(T_r)}{(v_r)^2} - \frac{T_r}{\Omega(T_r)} log\left(1 - \frac{\Omega(T_r)}{v_r}\right)$$

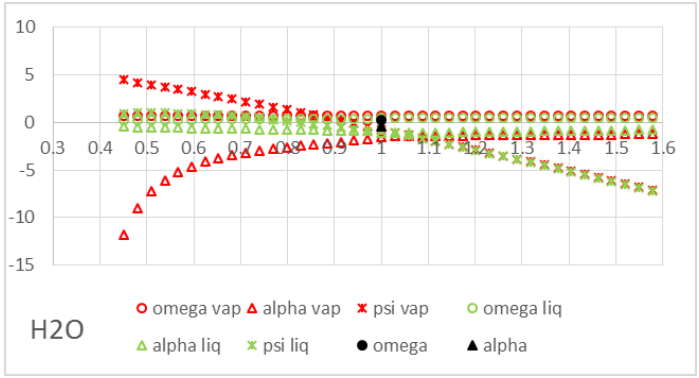
$$g_r = 2\frac{A(T_r)}{v_r} - T_r\, log\left(1 - \frac{\Omega(T_r)}{v_r}\right) - T_r\, log(v_r) + \Psi(T_r)$$

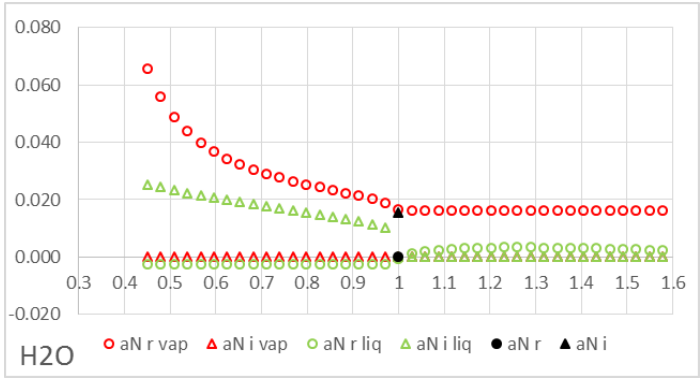
Phase Equilibrium – Fluid Components

Fluid NIST database		Fluid Derived	
Methane	ch4	C3-C5	c4h10
Ethane	c2h6	i-Pentane	c5h12-i
Propane	c3h8	m-Xylene	c8h10
n-Butane	c4h10	Aro C6-C14	c10h8
i-Butane	c4h10-i	Sat C6-C14	c10h22
n-Pentane	c5h12	n-Undecane	c11h24
Benzene	c6h6	n-Tridecane	c13h28
n-Hexane	c6h14	n-Tetradecane	c14h30
Toluene	c7h8	n-Pentadecane	c15h32
n-Heptane	c7h16	n-Hexadecane	c16h34
n-Octane	c8h18	n-Heptadecane	c17h36
n-Nonane	c9h20	n-Octadecane	c18h38
n-Decane	c10h22	Aro C15+	c18h12
n-Dodecane	c12h26	Aro C15+ A	c18h12
Carbon Dioxide	co2	Aro C15+ B	c18h12
Hydrogen Sulfide	h2s	Sat C15+	c19h40
Nitrogen	n2	n-Nonadecane	c19h40
Oxygen	o2	n-Eicosane	c20h42
Water	h2o	Resin	c38h59.5o.3n.4s.2
		Asphaltene	c53h62.6on.7s.6

Phase Equilibrium - Data

- Polarizability vs temperature & phase (a, aN r, aN i, alpha)
- Final molecule size correction vs temperature & phase (b, B, omega)
- Gibbs free energy term vs temperature & phase (F, psi)

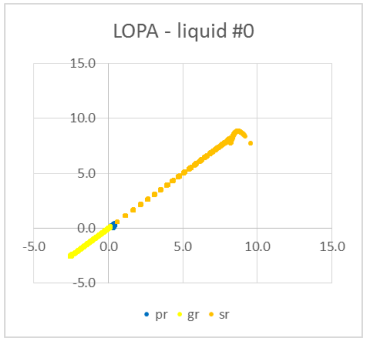


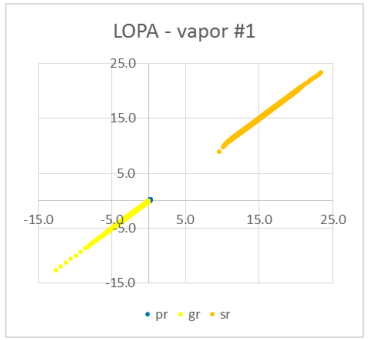


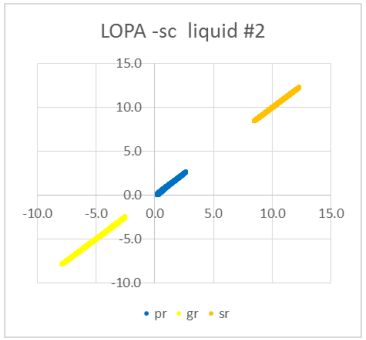
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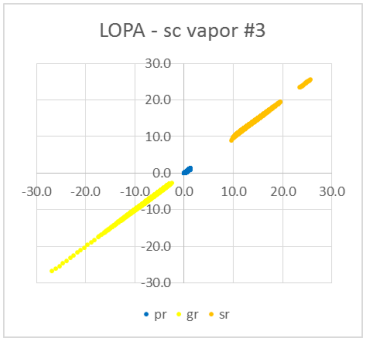
Phase Equilibrium - Data

- NIST fluid database & dimensionless type curves









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Phase Equilibrium – Basin Modeling

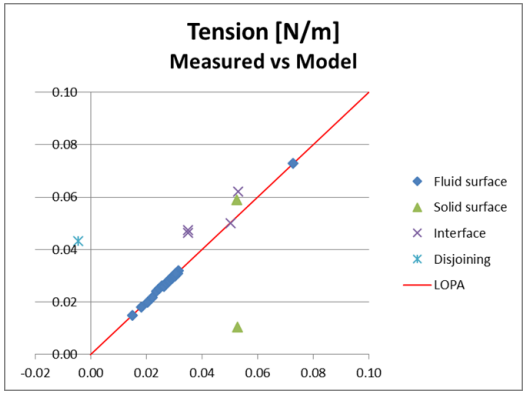
- Interfacial tension $\gamma_{s,j,m} = \gamma_{j,m} cos(\Theta_{s,j,m}) = \gamma_{s,m} - \gamma_{s,j}$

$$\gamma_{j,j+1} = \frac{1}{2}\sum_{m}^{J} sign_{j,m}^{up} \sum_{i}^{I}\sum_{l}^{L}\sum_{p}^{P}\sum_{q}^{Q} \frac{\partial G_{il,pq}^{j,m}}{\partial A_{j,m}} + \sum_{m}^{J} sign_{j+1,m}^{down} \sum_{i}^{I}\sum_{l}^{L}\sum_{p}^{P}\sum_{q}^{Q} \frac{\partial G_{il,pq}^{j+1,m}}{\partial A_{j+1,m}}$$

$$sign_{j,m}^{up} = \begin{cases} 1 & \forall\, m > j \because across \\ -1 & \forall\, m \le j \because same\ side \end{cases} \qquad sign_{j+1,m}^{down} = \begin{cases} 1 & \forall\, j+1 > m \because across \\ -1 & \forall\, j+1 \le m \because same\ side \end{cases}$$

$$G_{il,\mathrm{pq}}^{jk,mn} = \int_{V_{jk}^{min}}^{V_{jk}} \int_{0}^{V_{mn}} \varphi_{\mathrm{pq}}^{il} N_i N_l \, dV dV$$

$$\int_{V_{jk}^{min}}^{V_{jk}} \int_{0}^{V_{mn}} \frac{1}{r^6} dV dV = A_{jk,mn} \frac{\pi}{12\left(\delta_{jk}^{i}\right)^2}$$



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Phase Equilibrium – Basin Modeling

- Capillary & disjoining pressure $p_m = p_j - \Pi_{j-m}$

$$\Pi_{j-m} = \frac{\partial}{\partial \delta^{il}} \sum_{\alpha} x_{\alpha}^{vol} \int_{0}^{\infty} \frac{f^{\alpha}(\delta_p)}{2A_{j,m}} d\delta_p \sum_{i}^{I} \sum_{l}^{L} \sum_{p}^{P} \sum_{q}^{Q} \sum_{j \neq m} \left(G_{il,pq}^{j,m} - G_{ii,pq}^{j,m} + G_{li,pq}^{m,j} - G_{ll,pq}^{m,j} \right)$$

$$G_{il,\mathrm{pq}}^{jk,mn} = \int_{V_{jk}^{min}}^{V_{jk}} \int_{0}^{V_{mn}} \varphi_{\mathrm{pq}}^{il} N_i N_l \, dV dV$$

$A_{3,2} = A_{WF,NWF}$: $\frac{\partial}{\partial \delta^{il}} \int_{0}^{V_3} \int_{0}^{V_2} * \, dV dV = \frac{2}{r_{ci}} \int_{0}^{V_3} \int_{0}^{V_2} * \, dV dV$ Capillary bubble

$A_{4,3} = A_{NWA,WF}$: $\frac{\partial}{\partial \delta^{il}} \int_{0}^{V_4} \int_{0}^{V_3} * \, dV dV = \frac{4}{D_o} \int_{0}^{V_4} \int_{0}^{V_3} * \, dV dV$ Film thickness

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Phase Equilibrium – Basin Modeling

- Multi-component & multi phase distribution
- Fugacity

$$RTlog\left(\frac{\hat{\varphi}_i}{\hat{\varphi}_{i\,ref}}\right) = \int_0^p \left(\frac{\partial V_t^j}{\partial n_i^j}|_{T,n_{l\neq i}} - \frac{RT}{p}\right)_T dp$$

$$= -\left(a_{jj}^l + (1-x_{ij})a_{i-jj}^l + x_{ij}a_{ii-jj}^l\right)\frac{1}{V_j}$$

$$+\left(\frac{1}{V_{j-1}}a_{i-jj-1}^l + \frac{1}{V_{j+1}}a_{i-jj+1}^l\right)log(V_j)$$

$$-\left(a_{jj}^c + (3-x_{ij})a_{i-jj}^c + x_{ij}a_{ii-jj}^c\right)\left(\frac{1}{V_j}\right)^{1/3}$$

$$-RTlog\left(1-\frac{B_j}{V_j}\right)(1+V_j\,B_{term}) - RTlog\left(\frac{p_jV_j}{RT}\right)$$

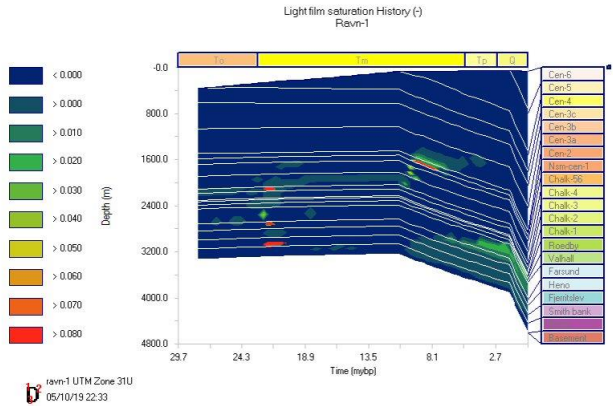
$$B_j(T) = \begin{cases} \sum_i x_{ij}B_{ij}(T) & mole\ arithmetic\ average\ of\ B_{ij} \\ \frac{\sum_i x_{ij}v_{ci}}{\sum_i \frac{x_i}{\omega_i(T)}} & critical\ volume\ hyperbolic\ average\ of\ B_{ij} \end{cases}$$

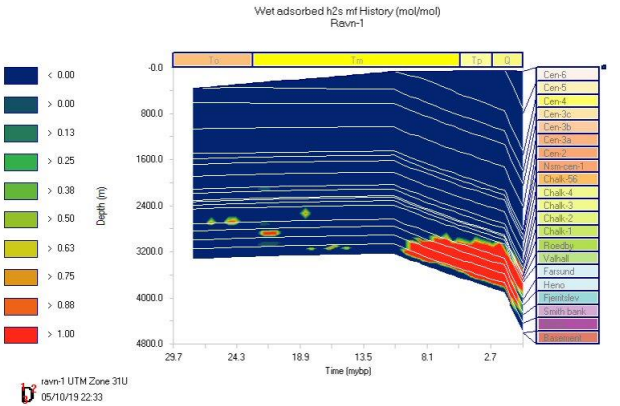
$$B_{term} = \begin{cases} \frac{B_{ij}-B_j}{{B_j}^2} & mole\ arithmetic\ average\ of\ B_{ij} \\ \rho_c\left(\frac{v_{ci}}{B_j}-\frac{1}{\omega_{ij}}\right) & critical\ volume\ hyperbolic\ average\ of\ B_{ij} \end{cases}$$

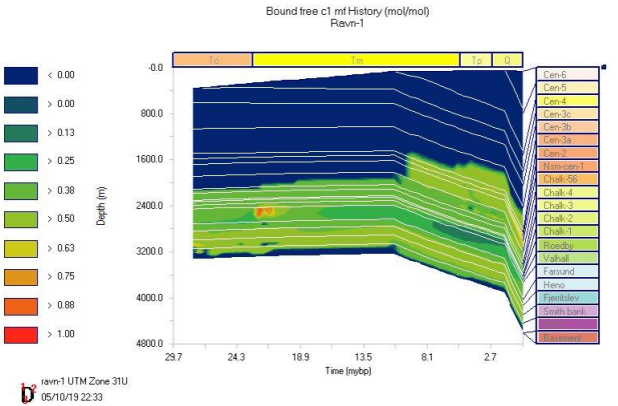
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Phase Equilibrium – Basin Modeling

- Multi-component & multi phase distribution







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Phase Equilibrium – Basin Modeling

- Transport properties
  - Viscosity
  - Thermal conductivity
  - Thermal expansivity
  - Compressibility
  - Heat capacity

$$\mu=\frac{5\pi}{32}\frac{l_k\bar{v}}{v}\frac{1}{mw} \qquad \bar{v}=\sqrt{\frac{8\ RT}{\pi\ mw}} \qquad \delta=\sqrt[3]{\frac{3B}{4\pi}}$$

$$\alpha=\frac{\partial p}{\partial T}\Big|_v \beta \qquad \beta=1/v/\frac{\partial p}{\partial v}\Big|_T$$

$$k_t=\frac{1}{3}T\frac{\partial s}{\partial T}\Big|_v\frac{l_t\bar{v}}{v} \qquad l_k=\frac{v}{\sqrt{2}\pi N_A\delta^2}f_j \qquad l_t=\frac{v}{\sqrt{2}\pi N_A\delta^2}g_j$$

$$c_v=T\frac{\partial s}{\partial T}\Big|_v\frac{1}{mw} \qquad c_p=c_v+Tv\left(\frac{\partial p}{\partial T}\Big|_v\right)^2\beta\frac{1}{mw}$$

Phase	*viscosity f*	*tconductivity g*
Liquid	$2exp\left(\frac{3}{2}(T_c/T-1)\right)$	$12\left(1+\frac{3}{2}(T/T_c-1)\right)$
Vapor	1	1

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Phase Equilibrium – Basin Modeling

- Free phase viscous drag
- Hydraulic radius

$$\bar{v}_j - \overline{v_m} = -\frac{1}{2} R_{H\,j,m}^2 \frac{\tau_j}{\mu_j}\left(\nabla p_j - \rho_j \bar{g}\right)$$

$$R_H^{WF} = \frac{V_{WF}}{A_{NWA,WF}} = \frac{V_3}{A_{4,3}}$$

$$R_H^{NWF} = \frac{V_{NWF}}{A_{WF,NWF}} = \frac{V_2}{A_{3,2}}$$

$$R_H^{BF} = \frac{V_{BF}}{A_{NWFBF}} = \frac{V_1}{A_{2,1}}$$

$$\tau = \left(\frac{L}{L_{streamline}}\right)^2$$

$$\tau_{hor} = \left(\frac{L_{surf} A_r^{1/3}}{L_{surf}} \frac{1}{\frac{\pi}{2}} \frac{\pi}{1-\phi} \frac{\pi}{6}\right)^2 = \left(\frac{1}{3} \frac{A_r^{1/3}}{1-\phi}\right)^2$$

$$\tau_{vert} = \left(\frac{L_{surf} A_r^{-2/3}}{L_{surf}} \frac{1}{\frac{\pi}{2}} \frac{\pi}{1-\phi} \frac{\pi}{6}\right)^2 = \left(\frac{1}{3} \frac{A_r^{-2/3}}{1-\phi}\right)^2$$

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Organic Kinetics - Background

- Pseudo components
  - Inconsistent stoichiometry
  - Kinetic data vary with paleo environment
  - No intermediary solid component
  - Little connection to present day biochemistry

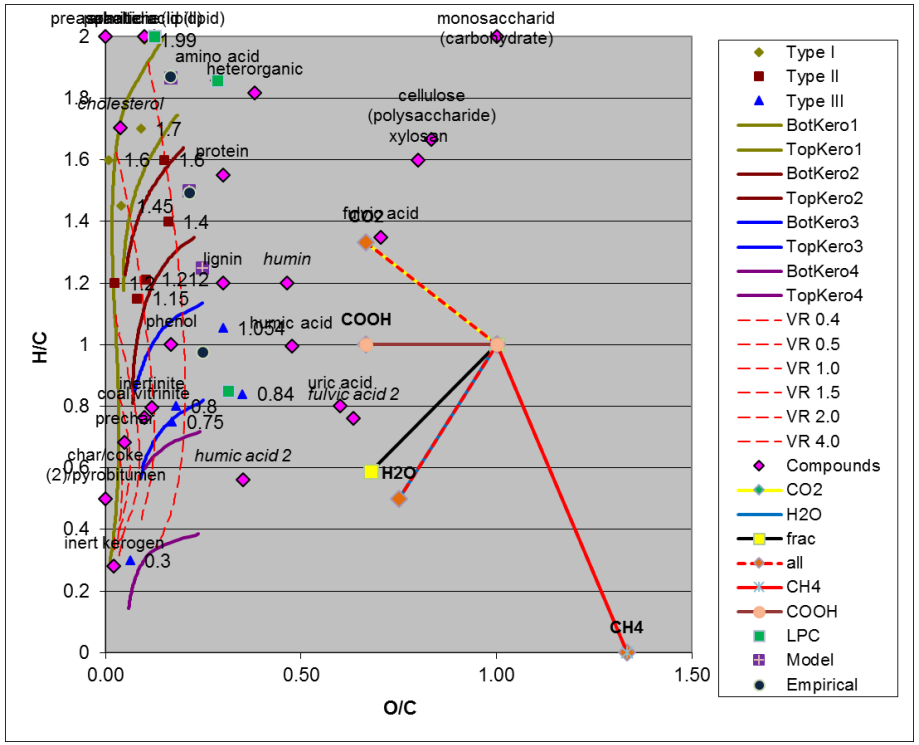
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Organic Kinetics – Minerals

Lipid	HOOC(CH2)14CH3
Protein	C400H620N100O120PS
Carbohydrate	(C6H10O5)n
P-Coke	CH.68S.04
Coke	CH.67
Lignite	CH.849N.015O.211
Graphite	C
Coal Vitrinite	C102H78O10N2
Humin	C56.1H5.5O34.7N3.7S0.4
Phenol	C6H5OH
Lignin	C10H12O3
Cholesterol	C27H46O
Humic Acid	C187H186O89N9S
Fulvic Acid	C135H182O95N5S2
Amino Acid	H2NCHRCOOH (R - C5H11)
Uric Acid	C5H4N4O3

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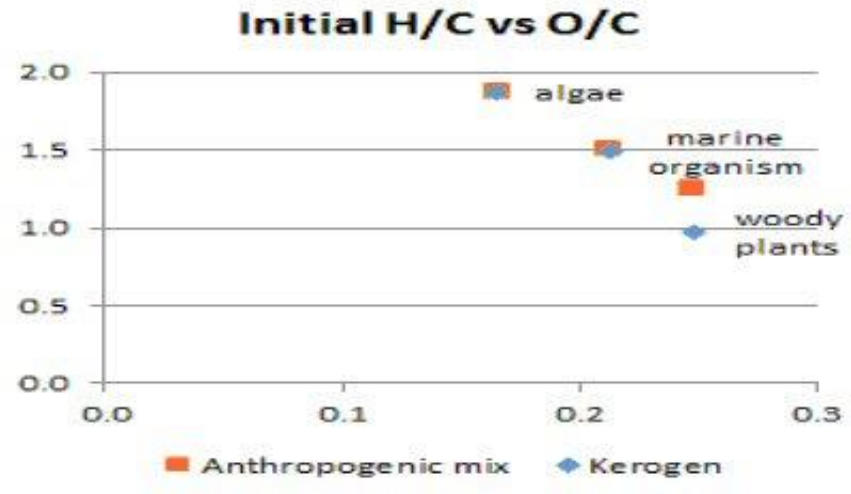
Organic Kinetics – van Krevelen Diagram



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Organic Kinetics - Kerogen

- Kerogen components
  - Lipid
  - Protein
  - Carbohydrate



	I	II	III
	algae	marine organism	woody plants
Lipid	76%	53%	35%
Protein	14%	4%	0%
Carbohydrate	10%	43%	65%

1 2 3 123D Technology

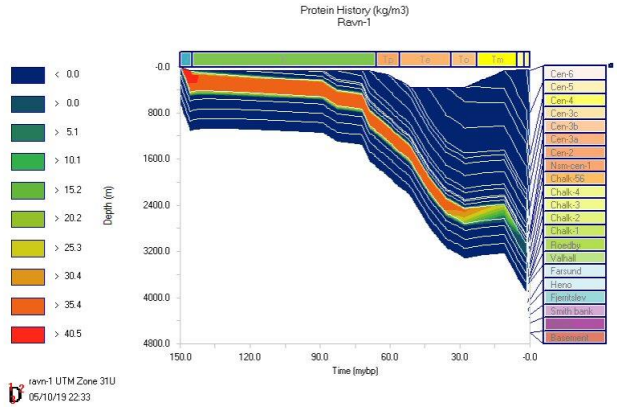
Organic Kinetics - Reactions

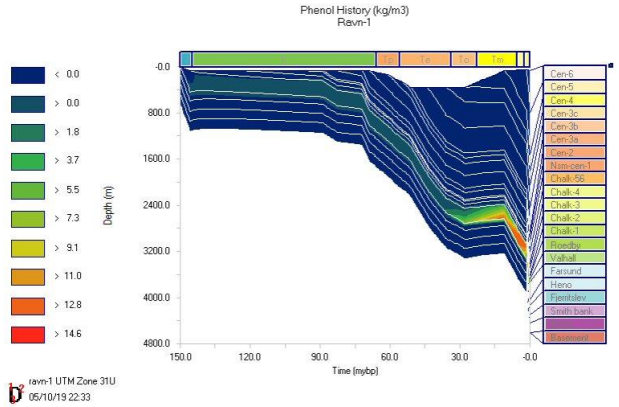
Humic Acid	-> 0.20 * C Vitrinite + 2.32 * Humin + 36.21 * C1 + 0.07 * H2S + 6.35 * H2O
Fulvic Acid	-> 23.35 * Coke + 0.56 * Humic Acid + 7.76 * CO2 + 15.88 * H2S + 2.73 * H2O
Amino Acid	-> 0.07 * Cholesterol + 0.09 * ASPH + 0.49 * N2 + 1.80 * H2O
C Vitrinite	-> 93.18 * Coke + 3.85 * C1 + 5.00 * CO2 + 1.00 * N2
Humin	-> 35.42 * Graphite + 0.39 * Lignin + 16.76 * CO2 + 0.40 * H2S + 1.85 * N2
Phenol	-> 2.50 * Graphite + 0.02 * ARO15+ + 0.14 * SAT15+ + 0.50 * CO2
Lignin	-> 7.03 * Graphite + 0.29 * Phenol + 1.21 * C1 + 2.71 * H2O
Cholesterol	-> 1.00 * Phenol + 0.24 * ARO15+ + 0.88 * SAT15+
Lipid	-> 0.42 * Phenol + 0.43 * Cholesterol + 1.83 * C1 + 1.15 * H2O
Protein	-> 36.77 * Phenol + 9.59 * Amino Acid + 1.15 * NSO + 1.32 * ASPH + 44.71 * N2 + 62.85 * H2O
Carbohydrate	-> 0.01 * C Vitrinite + 0.04 * Fulvic Acid + 0.001 * C1 + 0.08 * CO2 + 0.005 * N2 + 1.32 * H2O
C2	-> 0.50 * Graphite + 1.50 * C1
C3-5	-> 0.86 * Coke + 0.007 * C1 + 1.57 * C2
ARO6-14	-> 3.87 * Coke + 0.03 * C1 + 0.54 * C2 + 1.07 * C3-5
SAT6-14	-> 0.60 * Coke + 1.40 * C1 + 0.57 * C3-5 + 0.62 * ARO6-14
ARO15+	-> 11.88 * Coke + 0.10 * C1 + 0.39 * C3-5 + 0.42 * ARO6-14
SAT15+	-> 0.60 * Coke + 1.40 * C1 + 1.39 * SAT6-14 + 0.18 * ARO15+
NSO	-> 1.60 * ARO6-14 + 0.49 * SAT6-14 + 0.95 * ARO15+ + 0.09 * SAT15+ + 0.13 * CO2 + 0.16 * H2S + 0.19 * N2
ASPH	-> 10.75 * Coke + 1.37 * ARO15+ + 0.46 * NSO + 0.26 * CO2 + 0.55 * H2S + 0.73 * N2

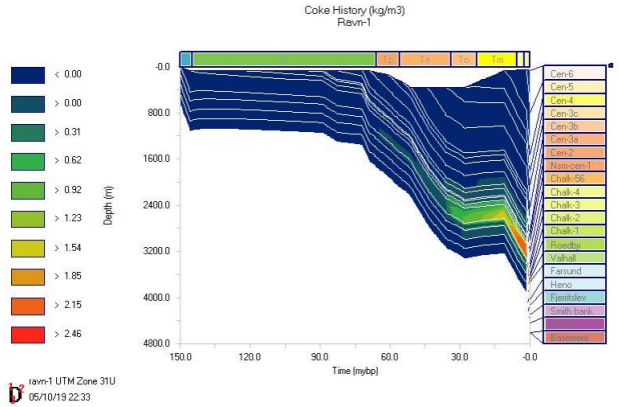
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Organic Kinetics – Basin Modeling

- Mineral evolution
  - Protein
  - Phenol
  - Coke







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Issues

- Data refinement
- Speed
- Stability

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Issues – Data Refinement

- Fluid data
  - Substitute dimensionless type curves (21) with NIST type fluid database (19)
  - Kinetics (xi, E & A)
- Mineral data
  - LN dist (α & β^2)
  - Elasticity (G & ν)
  - Viscosity (μ & T)
  - Electrical (μ & ε)
  - Kinetics (xi, E & A)

Issues – Speed

Precision 7740® 16 proc 2.4 Ghz 128 GB	**West Greenland Gen&Mig 2P**	**DCG Gen&Mig MP**	**DCG Gen&Mig 2P**	**IAJK-24 Gen&Mig MP**	**IAJK-24 Gen&Mig 2P**	**Ravn-1 Gen&Mig MP**	**Ravn-1 Gen&Mig 2P**
Study area	312 km * 432 km (~135000 km^2)	90 km * 65 km (~6000 km^2)	90 km * 65 km (~6000 km^2)	50 km * 1 km (50 km^2) 2D	50 km * 1 km (50 km^2) 2D	1D	1D
Components (solid+fluid)	8+5	21+13	9+5	21+13	9+5	21+13	9+5
Horizontal gridcells	20x20=400	21x19=399	21x19=399	40	40	1	1
Avg. cell size	16 km * 22 km	4.3 km * 3.4 km	4.3 km * 3.4 km	1.25 km * 1 km	1.25 km * 1 km	1 km * 1 km	1 km * 1 km
Basin thickness	1 - 7 km	4 - 7 km	4 - 7 km	4 -7 km	4 -7 km	4.4 km	4.4 km
Vertical gridcells	26	74	74	74	74	73	73
Study time	152 ma	290 ma	290 ma	290 ma	290 ma	290 ma	290 ma
Execution time	5.6 hours	9.1 days	8.5 days	1.7 days	1.9 hours	1 hour	8 min

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Issues – Task Timing

- Hardware
  - Parallel
    - CPU
    - GPU
- Key task
  - Compaction
  - Phase density
  - Phase distribution
  - Transport properties

```
Task Timing:
  TT_MODELINI                          time (sec)       1.00
  TT_GRIDGEN                           time (sec)       1.00
  TT_GRIDVAR                           time (sec)       1.00
  TT_GRIDADMIN                         time (sec)       2.00
  TT_SETUP                             time (sec)      39.00
  TT_SOLVE_EXCESSPRESSAT               time (sec)      11.00
  TT_SOLG_EXCESSPRESSAT                time (sec)       6.00
  TT_SOLG_FLUIDPRES                    time (sec)       2.00
  TT_SOLVE_ROCKPOS                     time (sec)     209.00
  TT_SOLVE_ROCKSYSTEM                  time (sec)       9.00
  TT_SOLG_ROCKSYSTEM                   time (sec)       5.00
  TT_SOLVE_TEMPERATURE                 time (sec)       1.00
  TT_SOLG_TEMPERATURE                  time (sec)       2.00
  TT_MP_ANTE                           time (sec)       1.00
  TT_MP_SETUP                          time (sec)      43.00
  TT_MP_INITIAL                        time (sec)       1.00
  TT_MP_DENSITY                        time (sec)     188.00
  TT_MP_KL_DIST_COEF                   time (sec)      95.00
  TT_MP_DIST_COEF                      time (sec)     177.00
  TT_MP_LM_DIST_COEF                   time (sec)      38.00
  TT_MP_LM_GIJ_FUN                     time (sec)       6.00
  TT_MP_LM_FUN                         time (sec)       1.00
  TT_MP_LM_DFUN                        time (sec)      13.00
  TT_MP_LM_SOL                         time (sec)      72.00
  TT_MP_LM_DIST                        time (sec)       2.00
  TT_MP_POST                           time (sec)       7.00
  TT_UPDATE_ITE_ANTE_ROCK              time (sec)       5.00
  TT_UPDATE_SOL_EPRESSAT               time (sec)       1.00
  TT_UPDATE_SOL_TRANSPROP              time (sec)     202.00
  TT_UPDATE_SOL_PETROFLOWPROP          time (sec)       9.00
  TT_UPDATE_POST_ITE                   time (sec)       1.00
  TT_OUPPUT                            time (sec)     257.00
    Solve time (sec)    - Total:    230.00
    Elapsed time (sec) - Total:   1408.00
```

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Issues – Stability

- Loss of mass balance
- Remedies
  - Suppressing activity
    - Flow path fraction of cell length
    - Cracking fraction of component

Mass balance report

MMtons pr 1 km^2:

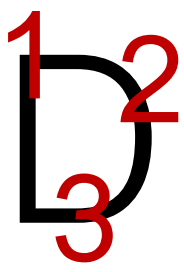
	Inside =	Boundary	+ Source	- Sink	Diff. %
Rock :	9502	9502			-4e-13
quartz :	3863.6	3863.6	0	0	-9.9e-05
Feldspar :	561.15	561.15	0	0	-0.00028
Albite :	275.71	275.72	0	0	-0.0012
Chlorite :	56.105	56.105	0	0	-0.00017
Illite :	523.79	523.79	0	0	9.5e-13
Smectite :	721.81	721.82	0	0	-0.00034
Kaolinite :	1159.3	1159.3	0	0	-7.3e-13
Calcite :	1161.6	1161.6	0	0	-5.1e-10
Dolomite :	68.38	68.38	0	0	2.9e-11
Siderite :	996.04	996.05	0	0	-0.00043
Pyrite :	8.8325	8.8326	0	0	-0.0005
Anhydrite :	105.62	105.62	0	0	5e-12
Humic Acid :	9.0162e-07	0	9.8766e-07	8.6121e-08	0.0089
Fulvic Acid :	1.2768e-05	0	1.4293e-05	1.5257e-06	0.007
Amino Acid :	0.01842	6.344e-07	2.1005	2.0821	-0.00085
Coke :	0.69454	1.3633e-12	0.69463	0	-0.013
Graphite :	1.2777	0	1.2777	0	-0.00057
C Vitrinite :	1.3242e-06	0	1.7856e-06	4.6151e-07	0.0074
Humin :	5.8762e-08	0	6.5189e-08	6.4324e-09	0.008
Phenol :	1.7326	1.5991e-06	5.7378	4.0044	-0.013
Lignin :	3.0457e-10	0	3.4929e-10	4.4185e-11	-0.15
Cholesterol :	1.2521	1.8438e-09	1.7756	0.5234	-0.0019
Lipid :	3.1187	5.2002	0	2.0804	-0.021
Protein :	0.025982	13.509	0	13.483	-0.0049
Carbohydrate :	2.7586	2.7591	0	1.9213e-05	-0.02
Kerogen :	7.2	21.5	4.6	18.2	-3.2
Carbon :	8.3	12.5			-34
C1 :	0.19496	-1.1871e-12	0.24316	0	-20
C2 :	0.063276	0	0.16061	1.9386e-06	-61
C3-5 :	0.24459	0	0.62082	1.8134e-05	-61
ARO6-14 :	0.017067	-7.4822e-18	1.3146	0.63775	-50
SAT6-14 :	0.18025	-2.1124e-18	0.45617	5.2612e-05	-60
ARO15+ :	1.5718	-1.662e-17	3.7208	7.9834e-05	-58
SAT15+ :	1.588	-3.2008e-20	2.0913	0.0036087	-24
NSO :	0.027792	-5.7154e-13	2.5495	1.7129	-32
ASPH :	0.031645	-9.1296e-13	2.492	2.4574	-0.12
CO2 :	0.77641	-1.0114e-15	1.0493	0	-26
H2S :	0.063625	-1.6449e-15	0.1585	0	-60
N2 :	1.8307	-2.6897e-09	2.2869	0	-20
H2O :	614.4	2107.3	0	0	-71

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Conclusion

- First principles model
  - Compaction
  - Phase equilibrium
  - Kinetics
- Issues
  - Data
  - Speed
  - Stability
- Remedy
  - Cooperation with stakeholders

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