Impact of Equation of State on Simulating CO_2 Pipeline Decompression

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CO_2 Properties and EoS for Pipeline Engineering

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Structure

1. Background
2. Equations of State
3. Impact on simulation of pipeline decompression
4. Conclusions

Structure

1. Background

Pipeline ductile fracture

Running fractures represent a threat to CO_2 pipelines

A ductile fracture will come to rest when the fluid pressure at the crack tip, P_t falls below the Crack Arrest Pressure, P_a.

Pipeline decompression

- At the rupture plane the fluid is exposed to ambient air
- Following the rupture, the rarefaction wave starts propagating along the pipe at the speed of sound
- The vapour phase emerges in the expansion wave reducing the mixture speed of sound
- Due to rapid cooling of the fluid in the decompression wave, the solid phase may also be released from the pipe

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Cubic Equations of State

Generalized cubic EoS

$$z^3-(1-B^*-uB^*)z^2+(A^*+\omega B^{*2}-uB^*-uB^{*2})z-A^*B^*-\omega B^{*2}-\omega B^{*3}=0$$

$$A^*=\frac{aP}{RT^2},\ B^*=\frac{bP}{RT}$$

EoS	*a*	*b*		*b*	
RK u=1, w=0	$0.42748\frac{R^2(T_c)^{2.5}}{P_c}$	$0.08664\frac{RT_c}{P_c}$	5 —	$0.08664\frac{RT_c}{P_c}$	
SRK u=1, w=0	$0.42748\frac{R^2(T_c)^{2.5}}{P_c}$	$0.08664\frac{RT_c}{P_c}$	5 —	$0.08664\frac{RT_c}{P_c}$	$a(T)=[1+$ —
PR u=2, w=-1	$0.45724\frac{R^2(T_c)^2}{P_c}$	$0.07780\frac{RT_c}{P_c}$	-	$0.07780\frac{RT_c}{P_c}$	$a(T)=[$
PR/G u=2, w=-1	$0.45724\frac{R^2(T_c)^2}{P_c}$	$0.07780\frac{RT_c}{P_c}$	-	$0.07780\frac{RT_c}{P_c}$	$a(T)=$

SAFT and PC-SAFT Equations of State

$$\frac{a^{res}(T,\ \rho)}{RT} = \frac{a(T,\ \rho)}{RT} - \frac{a^{ideal}(T,\ \rho)}{RT} = \frac{a^{ref}(T,\ \rho)}{RT} + \frac{a^{disp}(T,\ \rho)}{RT} = \frac{a^{hs}(T,\ \rho)}{RT} + \frac{a^{chain}(T,\ \rho)}{RT} + \frac{a^{assoc}(T,\ \rho)}{RT} + \frac{a^{disp}(T,\ \rho)}{RT}$$

The SAFT (Statistical Associating Fluid Theory) equation of state is written as a summation of residual Helmholtz free energy terms that occur due to different types of molecular interactions in the system under study.

Hard sphere term:	$\frac{A^{hs}}{RT} = \frac{4n - 3n^2}{(1-n)^2}$	Carnahan-Starling EoS for hard spheres
Chain term:	$\frac{A^{chain}}{RT} = (1-m)\ln\frac{1-0.5n}{(1-n)^3}$	based on Wertheim's TPT1
Association term:	$\frac{A^{assoc}}{RT} = \sum_{A=1}^{M}\left(\ln X^{A} - \frac{X^{A}}{2}\right) + \frac{1}{2}M$	based on TPT1
Dispersion term:	$\frac{A^{disp}}{RT} = \sum_{i=1}^{4}\sum_{j=1}^{9} D_{ij}\left(\frac{u}{kT}\right)^{i}\left(\frac{n}{\tau}\right)^{j}$	Alder equation from molecular dynamics

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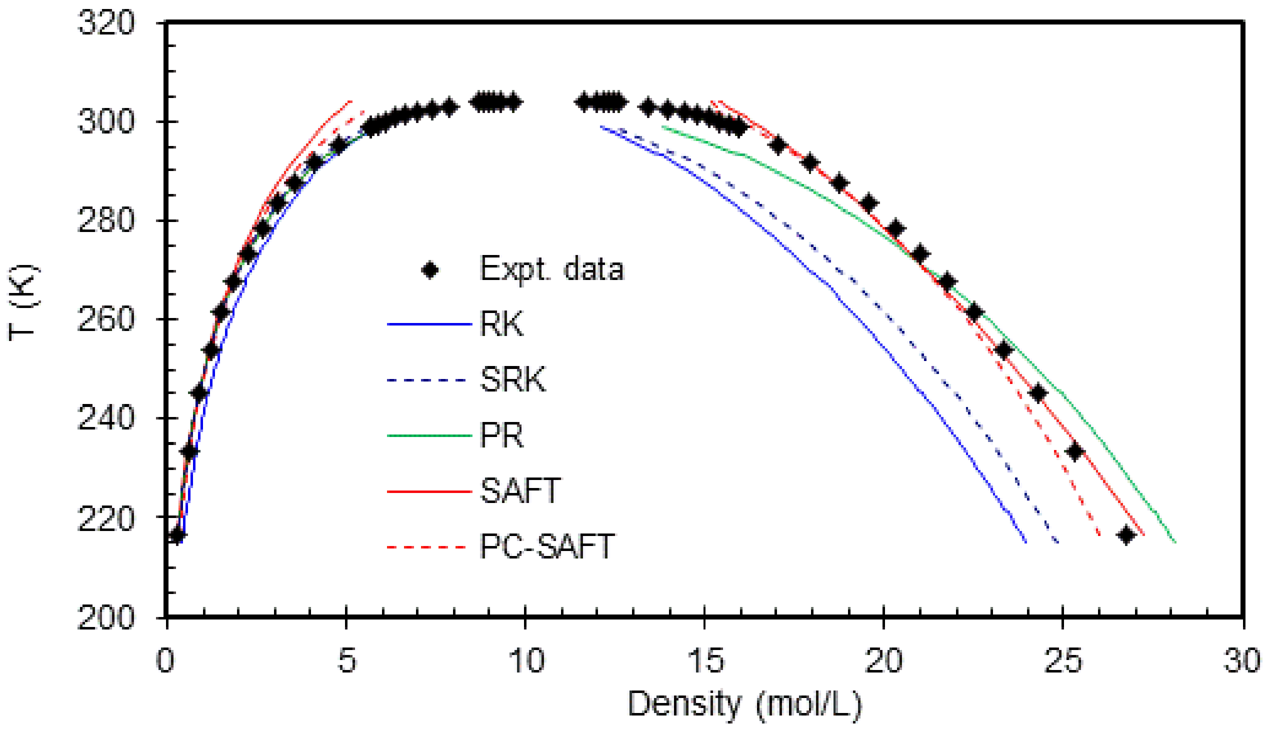
Saturated density predictions



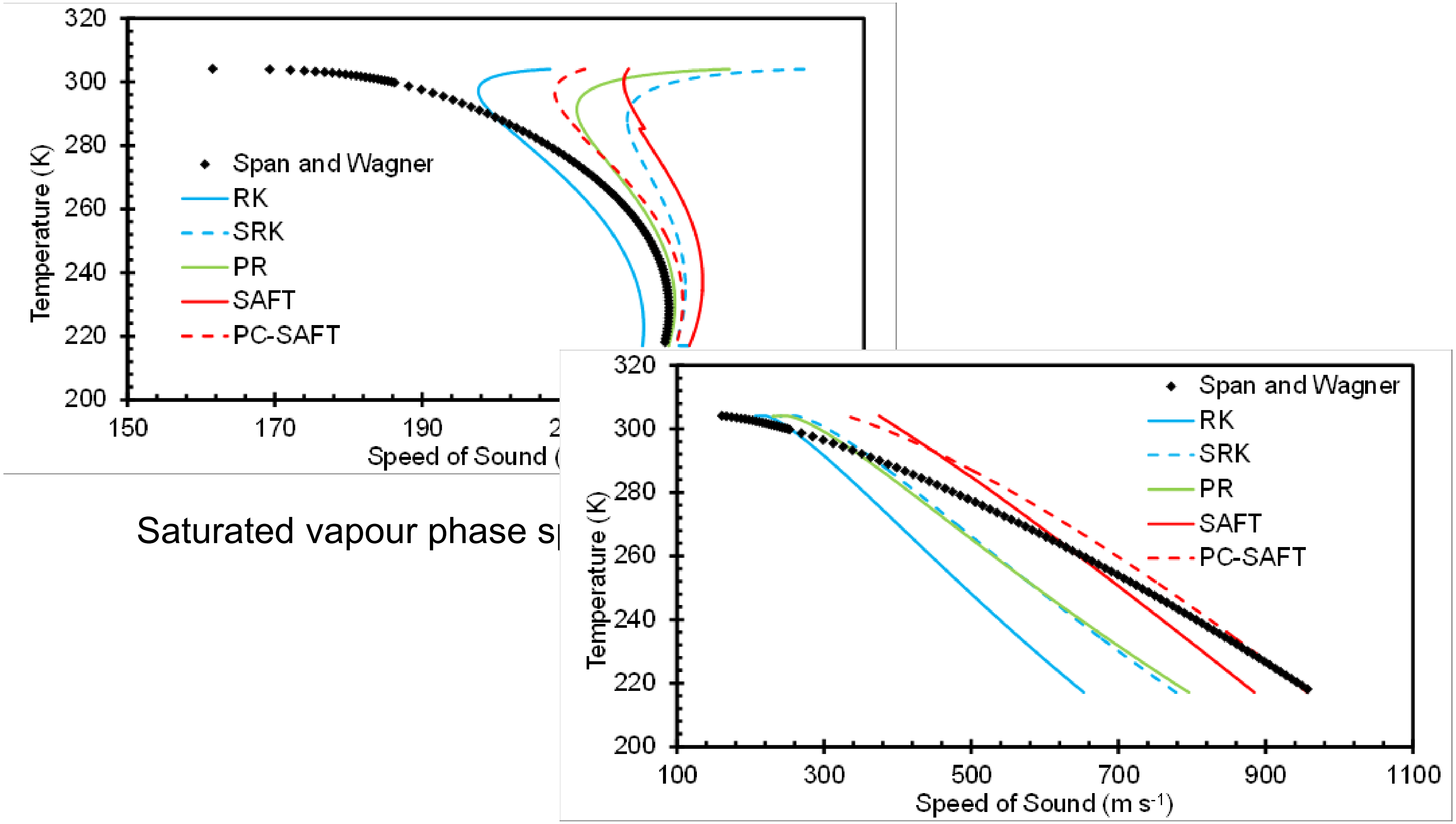
Saturated liquid and vapour density predictions
using the various Equations of State

Accuracy of derivative properties

	SAFT	PC-SAFT	RK	PR	SRK	Yokozeki
Density	1.81	1.14	6.25	4.89	5.97	3.35
Cv	6.37	3.77	9.96	3.94	8.80	58.75
Cp	11.09	3.53	10.35	4.54	3.35	28.76
Sound Speed	6.73	3.26	16.65	13.53	11.86	15.39
Joule-Thomson	113.11	44.20	75.70	102.08	66.65	85.62

Comparison of the predictive accuracy of EoS (AAD%) for important derivative properties.

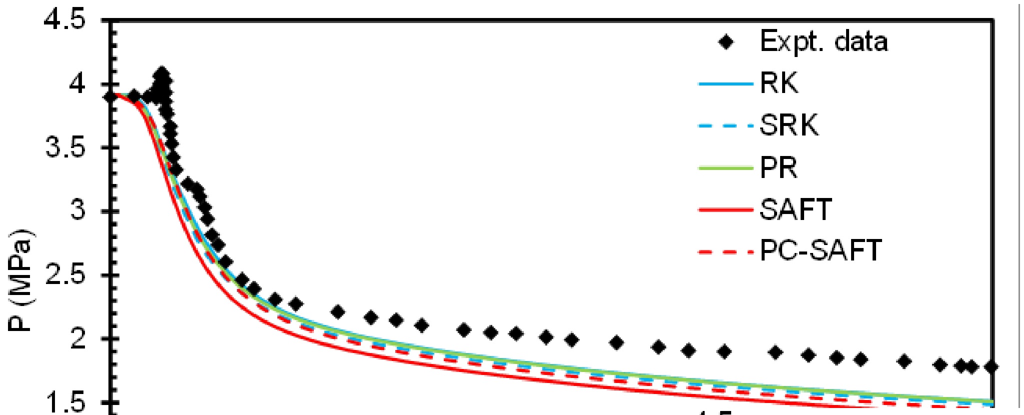
Speed of Sound predictions



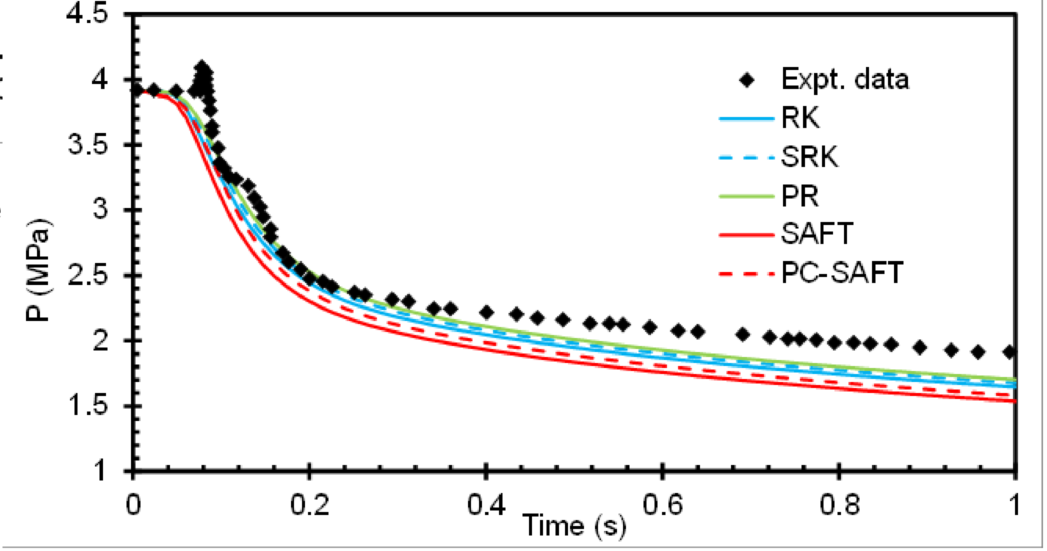
Saturated vapour phase s

Saturated liquid phase speed of sound

Vapour phase decompression

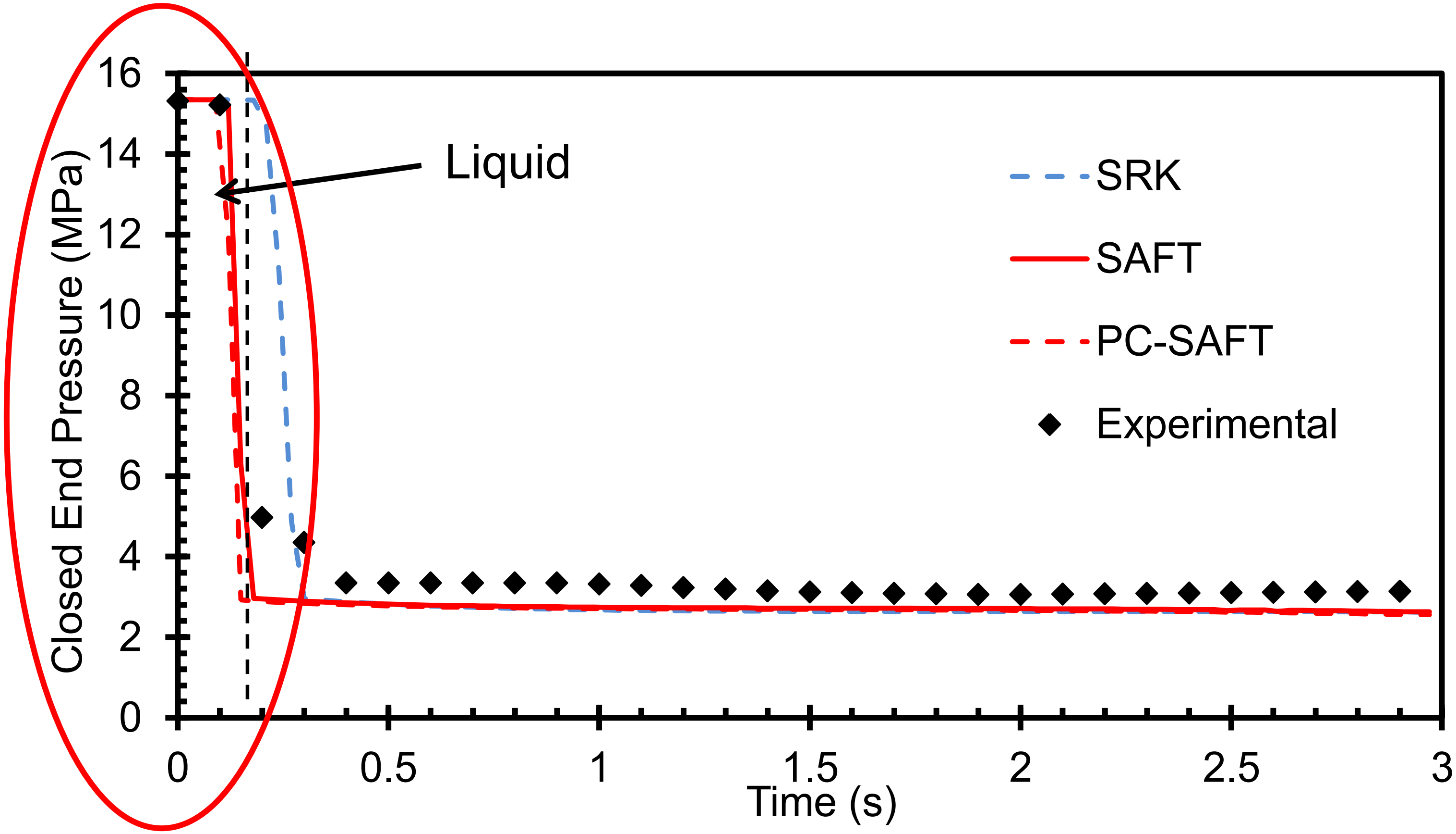


Pressure history during de
13.5 m from open



Pressure history during decompression
18 m from open end

Liquid phase decompression



Pressure history during decompression 143 m from open end

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- Accuracy of speed of sound in liquid predicted by even complex EoS remarkably low

- This greatly affects the modelling of the decompression wave, given that its front moves at the speed of sound

- Very little experimental data for dense phase speed of sound available for development of better EoS

- Results presented relate to pure CO_2 only, the little impure CO_2 data we have indicates that the same observations are true

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