

Dynamic flow of CO₂ in pipelines: Sensitivity to impurities

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Summary

This memo investigates the effect of impurities on the occurrence of two-phase flow in CO2-transport pipelines. The flow is modelled by a single-phase fluid-dynamical model and the simulation is interrupted at the first appearance of a bubble. The thermodynamical properties of the mixtures are described by the SRK equation of state with van der Waals mixing rules. A simplified pump model is used at the inlet of the pipe, while at the outlet, a simplified injection model mimics injection into a reservoir.

A test case is defined to simulate the load variation of a power plant during the day. The aim is to find in which conditions two-phase flow can occur, by varying the inlet temperature and the CO2-mixture composition concentration. A buried and a non-buried pipe are studied. We find that the CO2-mixture composition has an effect on whether two-phase flow will occur for a given inlet temperature. The environment of the pipe also has a strong effect.

Keywords	Fluid dynamics, thermodynamics, impurities, CO ₂ transport.
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1 Introduction

In CO₂ transport by pipeline, the massflow to be transported will vary with time, as well as the fluid properties. Each industrial site will produce varying quantities of CO₂, containing impurities depending on the site type and on the capture process. Besides, the different sites of a cluster sending CO₂ in a shared pipeline, will produce CO₂ with different properties and in varying quantities.

Impurities have an effect on the thermodynamical properties of the CO_2 mixture, in particular on the phase envelope. This plays a role in whether the flow will remain in single phase. The design should take into account the possible occurrence of two-phase flow, especially with corrosive phases like water. Two-phase flow may also lead to unstable flow (slug, vertical flows,...), and cause problems in compressors or pumps, etc.

Chaczykowski and Osiadacz [1] started to assess the effect of impurities in CO_2 on the flow in pipelines. The present work systematises that study and investigates the effect of the fluid properties on the flow during a slow transient. The test case run in the present work is inspired from the varying load of a power plant. It is not in the scope of this work to study multiphase flow. Therefore the flow is stopped when multiphase flow occurs.

Some of the present results were presented as a poster at the 7th Trondheim CCS Conference.

2 The models

The single-phase flow is modelled by the Euler equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \left(\rho u\right)}{\partial x} = 0, \tag{1}$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \tau_w, \tag{2}$$

$$\frac{\partial \left(\rho \left(e + \frac{1}{2}u^{2}\right)\right)}{\partial t} + \frac{\partial \left(\rho \left(e + \frac{1}{2}u^{2}\right)u + pu\right)}{\partial x} = Q_{w},$$
(3)

where ρ is the fluid density, *u* is the velocity, *p* is the pressure and *e* is the internal energy. The source terms τ_w and Q_w are the wall friction and the heat transfer from the wall to the fluid, respectively. The fluid thermodynamical state is described by the Soave-Redlich-Kwong (SRK) equation of state with van der Waals mixing rules (see for example [2, p.75, 85]). The physical properties, like the viscosity, the heat capacity and the heat conductivity are evaluated using the TRAPP model, which is a corresponding-states model [3, 4].

The Haaland approximation of the Colebrook correlation [5] gives the Darcy friction factor

$$f_D = \frac{64}{\text{Re}} \qquad \qquad \text{if } \text{Re} < 2000, \qquad (4)$$

$$\frac{1}{\sqrt{f_D}} = -1.8 \log_{10} \left[\left(\frac{\varepsilon/D}{3.7} \right)^{1.11} + \frac{6.9}{\text{Re}} \right] \qquad \text{if } \text{Re} \ge 2000, \tag{5}$$





and the friction term is given by the Darcy-Weisbach equation

$$\tau_w = f_D \cdot \frac{\rho u^2}{2D}.\tag{6}$$

For the heat source term Q_w , a transient wall temperature model is used, which is able to simulate the heat transfer in the pipe material and in the soil. The heat transfer from the surrounding atmosphere is given by

$$Q_{\rm atm} = h_{\rm atm} (T_{\rm atm} - T_{w,o}), \tag{7}$$

where $T_{w,o}$ is the pipe-wall or soil temperature in contact with the atmosphere, T_{atm} is the atmospheric temperature, and h_{atm} is the heat transfer coefficient between the pipe-wall or the soil and the atmosphere. The heat transfer between the fluid inside the pipe and the pipe wall is given by

$$Q_w = h_f (T_{w,i} - T_f), (8)$$

where $T_{w,i}$ is the pipe-wall temperature in contact with the fluid, T_f is the fluid temperature and h_f is the heat-transfer coefficient between the fluid and the pipe wall. h_f is given by the Nusselt number, which is found using the Dittus-Boelter correlation [6, 7]

$$Nu = 0.023 Re^{0.8} Pr^{0.4}, (9)$$

where Nu is the Nusselt number, Re is the Reynolds number and Pr the Prandtl number. The geometry of the pipe and the soil are assumed to be annular.

At the inlet boundary condition, a pump is basically modelled by imposing the massflow and the fluid temperature, while the pressure is extrapolated from the pipe. At the outlet, the boundary condition is designed to mimic injection into a reservoir. Since the vertical flow is not modelled, the equivalent reservoir pressure is adjusted to the terrain altitude. The injected massflow is then, similarly to the model used in the Vedsted pipeline simulation [8], given by

$$\dot{m} = \left(p_{\text{pipe}} - p_{\text{reservoir}}\right)k_{\text{i}},\tag{10}$$

where the reservoir pressure $p_{\text{reservoir}}$ and the injectivity coefficient k_i are fixed. Then, the mass-flow is imposed, while the thermodynamical state is extrapolated.

3 Case study

3.1 CO₂ mixtures studied

In the present work, we have looked at the flow of binary mixtures of CO_2 with various impurities. The phase diagrams of several mixture are shown in Figure 1.

- CO₂–N₂ mixture in Figure 1a.
- CO₂–O₂ mixture in Figure 1b.
- CO₂–CH₄ mixture in Figure 1c.





- CO₂–H₂S mixture in Figure 1d.
- CO₂–H₂O mixture in Figure 1e.

Note that in the single-phase region (above the equilibrium curve), the temperature increases from right to left. On the CO₂–H₂O mixture phase diagram, also note the areas where a liquid water-rich phase exists. At higher water concentration (Figure 1f), the two areas with water-rich phases merge. The new area is denoted by (φ) in the Figure. Since the area (φ) stretches over the critical point for CO₂, the second phase is either vapour or liquid CO₂.

3.2 Case definition

We study a flat 50 km-long pipeline, with 1.27 cm wall thickness and 20 cm inner diameter. When the pipe is buried, the soil is a cylinder with a diameter of 1.27 m. The atmospheric temperature is 20 °C. The equivalent reservoir pressure at well head is 60 bar and the injectivity coefficient 2.4×10^{-5} kg s/Pa. The physical properties of the pipe and the soil are summarised in Table 1.

Table 1: Physical properties of the pipe and soil

	Pipe	Soil
Density (kg/m^3)	7850	1800
Heat capacity $(J/(kgK))$	470	1000
Heat conductivity $(W/(mK))$	45	2.6

The pipe flow, as well as the wall and soil temperatures, are brought to steady state, with a massflow of 60 kg/s at a given inflow temperature. Then, the massflow is varied at the inlet according to Figure 2. This is thought to reproduce the load variation of a power plant over one day. We then check if the flow remained in single phase over the whole cycle, or if boiling occurred.

4 Results

4.1 Plots

As an example, the pipeline pressure-density profiles are plotted in the phase diagram, for different concentrations of N_2 in CO₂ (Figure 3). The profile denoted by a (A) corresponds to the initial steady state. The profile denoted by a (B) correspond to the state just before increasing the massflow again. The profile is plotted both in the case of the buried pipe and in the case of the non-buried pipe. Boiling occurs when the outlet of the pipe goes under the equilibrium line.

4.2 Results for various compositions and temperatures

The test case has been run with different binary mixtures, amount of impurities, and inlet temperatures. Then, it was determined if the flow had remained in single phase during the whole cycle,







Figure 1: Phase diagram of different mixtures









Figure 2: Massflow at the pipe inlet over one day.



Figure 3: Pressure-density profile for the CO₂-N₂ mixture at 31 °C

or if boiling happened. The results are shown in Tables 2 and 3. If the flow remains single-phase, it is indicated by a \checkmark , and by a \thickapprox if there was boiling.

Impurities have an effect on whether the mixture boils or not. In the case of the buried pipe, there will not be boiling for pure CO₂ for an inlet temperature of $38 \,^\circ$ C or less. However, for O₂ and N₂ at 1 mol-%, boiling occurs down to $36 \,^\circ$ C. For N₂, the impurity concentration was pushed further, with increasing effect on boiling. At 5 mol-%, boiling happened for an inlet temperature down to $26 \,^\circ$ C. For CH₄, H₂S and H₂O, no significant effect is observed for the amounts of impurities tested here. This is expected, since the phase envelopes (Figure 1) were little changed by the amount of impurities. However, as shown on Figure 1f, the areas with liquid-water phase are growing with the amount of H₂O, and finally merging above the vapour–liquid equilibrium line. Thus, already at 0.5 mol-%, liquid water would be present even at initial state.

There is a significant difference between the results for the buried and for the non-buried pipes. In general, the non-buried pipe only tolerates a much lower inlet temperature than the buried pipe. The buried pipeline has more resistance to heat transfer, therefore the fluid remains at higher temperature. One could thus expect more boiling in the buried pipe. One possible reason



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	C	O_2 O_2 Molar fraction of impurity								
								5 0.0	 1	
		10W		поw	0.001	0.002	2 0.00	0.0	l 	
	35	°C ✓	3	5°C	v	 Image: A second s	 Image: A set of the set of the	\checkmark		
	36	5°C ✓	. 3	6°C	v	 Image: A second s		X		
	37	°C ✓	. 3	7°C			X	X		
	38	S°C ✓	3	8°C	×	×		×		
	39	о°С 🗡	3	9°C	*	<u>× ×</u>				
		(a) CO ₂		(b) CO ₂ –O ₂						
	N_2	Mola	r fractio	tion of impurity			N ₂ Mol		r frac	
-	Inflow	0.001	0.002	0.005	5 0.01		Inflow	0.02	0.05	
	35°C	\checkmark	\checkmark	\checkmark	\checkmark	_	25°C	\checkmark	\checkmark	
	36°C	\checkmark	\checkmark	\checkmark	×		26°C	\checkmark	×	
	37°C	\checkmark	\checkmark	×	×		:	:	÷	
	38°C	×	×	×	×		33°C	\checkmark	×	
	39°C	×	×	×	×		34°C	×	×	
		(c)	CO ₂ –N ₂				(d)	CO ₂ –N ₂		
CH ₄	Mola	r fraction	of imp	urity	. <u>—</u> н	H ₂ S Molar fraction of impurity				urity
т. с	0.001	0.002	0.005	0.01	Inf	low	0.001	0.002	0.005	0.01
Inflow	0.001									/
Inflow 35°C	0.001		 Image: A start of the start of	\checkmark	35	б°С	\checkmark	 Image: A second s	\checkmark	 Image: A second s
Inflow 35 °C 36 °C	✓ ✓	✓ ✓ ✓	✓ ✓	<i>\</i>	35 36	5°C 5°C	\checkmark	<i>\</i>	✓ ✓	<i>\</i>
Inflow 35 °C 36 °C 37 °C	✓ ✓ ✓	✓ ✓ ✓	✓ ✓ ★	✓ ✓ ✓	35 36 37	5°C 5°C 7°C				
Inflow 35 °C 36 °C 37 °C 38 °C	✓ ✓ ✓ ★	✓ ✓ ✓ ★	✓ ✓ ★ ★	✓ ✓ ✓ ★	35 36 37 38	S°C S°C V°C S°C	✓ ✓ ✓ ★	√ √ ✓ ★	✓ ✓ ★	✓ ✓ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	✓ ✓ ✓ ★	✓ ✓ ✓ ×	✓ ✓ × ×	✓ ✓ ✓ ★	35 36 37 38 39	5°C 5°C 7°C 5°C 5°C	√ √ × ×	√ √ × ×	✓ ✓ ★ ★	✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ★ CO ₂ -CH ₄	✓ ✓ × ×	✓ ✓ ★ ★	35 36 37 38 39	5°C 5°C 7°C 5°C 5°C	√ ✓ ✓ ★ (f) (✓ ✓ ★ CO ₂ -H ₂ S	✓ ✓ ★ ★	✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	✓ ✓ ★ ★ ★	✓ ✓ ✓ ★ Molar f	35 36 37 38 39 fraction	5°C 5°C 2°C 3°C 5°C 0°C	(f)	СО ₂ -H ₂ S	✓ ✓ ★ ★	✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	 ✓ ✓ × ×<	✓ ✓ ✓ ★ Molar f	35 36 37 38 39 fraction .0002	5°C 5°C 7°C 3°C 0°C	(f)	✓ ✓ СО2-H2S		✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	<pre></pre>	Molar 1	35 36 37 38 39 fraction .0002	3° C 3° C	(f)	СО ₂ -H ₂ S		✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	✓ ★ ★ ★ ₩ 0.00	Molar f	35 36 37 38 39 fraction .0002	3° C 3° C	(f) (purity 05 0.0	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓		✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	 ✓ ✓ ✓ ✓ ✓ ✓ (e) (✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓	✓ ★ ★ ₩ 0.00	Molar 1	35 36 37 38 39 fraction .0002	5°C 5°C 7°C 5°C 0°C 0°C	(f) (purity)5 0.0	✓ ✓ CO ₂ -H ₂ S		✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓		Molar 1	35 36 37 38 39 fraction .0002	5°C 5°C 7°C 3°C 0°C 0°C	(f)	СО ₂ -H ₂ S		✓ ✓ ★ ★
Inflow 35 °C 36 °C 37 °C 38 °C 39 °C	(e)	✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓		Molar f	35 36 37 38 39 fraction .0002	5°℃ 5°℃ 5°℃ 5°℃ 0°℃ 1 of im 0.000 √ √ ×	(f) (purity 05 0.0	СО ₂ -H ₂ S		✓ ✓ ★ ★

Table 2: Results for the buried pipe



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	CO ₂			O ₂ Molar fraction of impurity						
	Inflow			nflow	0.001	0.002	0.00	5 0.0	1	
	30°C ✓		3	0°C	 Image: A start of the start of	 Image: A start of the start of	 Image: A start of the start of	 ✓ 		
	31 °C ✓		3	1°C	\checkmark	\checkmark	✓	✓		
	32	°C ✓	3	2°C	\checkmark	√	 Image: A start of the start of	×		
	33	°C	3	3°C	X	×	X	×		
	34	34°C			*	<u> </u>				
		(a) CO ₂			(b)) CO ₂ –O ₂				
	N ₂	Mola	r fractio	n of im	purity		N ₂	Molar frac		
	Inflow	0.001	0.002	0.005	0.01	- <u> </u>	nflow	0.02	0.05	
	30°C	 Image: A second s	\checkmark	\checkmark	\checkmark		24°C	\checkmark	\checkmark	
	31°C	\checkmark	\checkmark	\checkmark	\checkmark	,	25°C	\checkmark	×	
	32°C	\checkmark	\checkmark	\checkmark	×		÷	:	:	
	33°C	×	×	X	×		30°C	\checkmark	×	
	34°C	×	X	×	×		31°C	×	X	
		(c)	CO ₂ –N ₂				(d)	CO ₂ –N ₂		
CH ₄	Mola	r fractior	n of imp	npurity H_2S Molar fraction of im				n of imp	urity	
Inflow	0.001	0.002	0.005	0.01	Inf	low (0.001	0.002	0.005	0.01
30°C	\checkmark	√	\checkmark	\checkmark	30	°C	\checkmark	\checkmark	\checkmark	\checkmark
31 °C	 Image: A second s	\checkmark	\checkmark	\checkmark	31	°C	\checkmark	\checkmark	\checkmark	\checkmark
32°C	\checkmark	\checkmark	\checkmark	\checkmark	32	°C	\checkmark	\checkmark	\checkmark	\checkmark
33°C	×	×	×	×	33	°C	×	×	×	×
34°C	×	×	×	×	34	°C	×	×	×	×
	(e)	CO ₂ –CH ₄					(f) C	$CO_2 - H_2S$		
		H ₂ C)	Molar f	raction	of imp	ourity			
		Inflo	w 0.00	001 0.	.0002	0.0005	5 0.00)1		
		30° (C 🗸	/	√	✓	 Image: A start of the start of			
		31° (c 🗸	/	\checkmark	\checkmark	 ✓ 			
		32° (C 🗸	/	\checkmark	\checkmark	✓			
		33° (c 🕻	t	×	×	×			
		30°C 31°C 32°C 33°C		(((✓ ✓ ★	✓ ✓ ★	× ×			

(g) CO₂-H₂O

Table 3: Results for the non-buried pipe





for that is that a higher temperature maintains a lower density, hence a higher fluid velocity and higher friction. This increases pressure drop and thus pressure in the pipe, which leads to less boiling. All in all, the pipe environment is very important in this test case. Note though that the effect of soil almost disappears for N_2 at 5 mol-%, where boiling happens close to the inlet temperature.

5 Conclusions

A single-phase flow simulation tool was used to assess the occurrence of boiling in a CO_2 pipeline during slow load variations. Different binary mixtures of CO_2 plus an impurity have been studied, with different concentrations of the impurity.

The occurrence of multiphase flow in CO_2 mixtures depends on the kind and amount of impurities present. The first and main reason is that the phase envelope is modified by the impurities – generally, boiling happens at higher pressure. The second reason is that the thermophysical properties change with impurities. For example, heat conductivity, viscosity or density. Heat exchange with the environment also plays a significant role.

Robust fluid- and thermodynamical simulation tools are needed to to predict the flow behaviour of the CO_2 during transients. In the present work, we have limited ourselves to the question whether two-phase flow will occur or not. The next step is to assess the effect of impurities in a two-phase flow, for example on cooling of the pipe.

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