TÍTULO DO TRABALHO:

MATHEMATICAL MODELLING AND COMPUTATIONAL IMPLEMENTATION OF THERMOPHYSICAL PROPERTIES AND MIXING RULES FOR DRILLING MUDS

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Resumo

Fluidos comumente usados na indústria de petróleo são misturas heterogêneas de hidrocarbonetos de diferentes tamanhos de cadeia, soluções aquosas e partículas sólidas. No caso de fluidos de perfuração, o conteúdo relativo de óleo, água e sólidos é escolhido para atingir um equilíbrio entre uma densidade alta o suficiente para suportar as altas pressões, mas com viscosidade apropriada para levar os carreados para a superfície. Recentemente, regulações ambientais têm um grande papel na definição de fluidos que possam ser usados como lamas, mudando a composição típica usada até então. Após a finalização da construção do poço, estes fluidos ficam confinados nos espaços anulares entre a coluna de produção e os revestimentos, e suas propriedades térmicas se tornam importantes durante a operação do poço porque influenciam a transferência de calor entre o fluido de produção e a formação rochosa, e sofrem expansão volumétrica devida às variações de temperatura. Neste trabalho, apresentamos resultados de uma biblioteca computacional dedicada ao cálculo de densidade, viscosidade, condutividade térmica e calor específico a pressão constante de diferentes tipos de fluidos de perfuração. Começando com componentes puros ou pseudo-puros, correlações empíricas para as propriedades de salmouras de NaCl e 1-hexadeceno são tomadas da literatura. A biblioteca é implementada em Python 2.7 para uso em um servidor que executa aplicativos de simulação para um importante operador da indústria de petróleo, e pesquisadores podem requisitar a geração de tabelas para uso em programas de simulação através de uma plataforma *web*. Todo o código foi desenvolvido por pesquisadores do nosso grupo, e programas de código aberto e comerciais são usados apenas para validação antes de lançar novas versões. Resultados preliminares são verificados com medições experimentais feitas no nosso laboratório de condutividade térmica, calor específico e densidade, e ajustes são propostas para as regras de misturas disponíveis.

Palavras-chave: propriedades termofísicas, fluidos de perfuração, termodinâmica de misturas, biblioteca computacional, Python 2.7

Abstract

Fluids commonly used in the oil industry are heterogenous mixtures of hydrocarbons of varying chain length, water solutions and solid particles. In the case of drilling muds, the relative contents of oil, water and solids are chosen to achieve a balance between a high enough value of density to support the high pressures but with appropriate viscosity to carry the cuttings from the bottom hole to the surface. In more recent years, environmental regulations play a large role in defining the fluids that can be used as muds, changing the typical formulation commonly used. After the well construction is finalized, these fluids become contained in the annular spaces between the production tubing and casings, and its thermal properties become important during operation of the well as they affect heat transfer between the operating fluid and the rock formation, also suffering volumetric expansion due to the temperature changes. In this work, we present results of a computational library dedicated to calculating density, viscosity, thermal conductivity and isobaric specific heat of different kinds of drilling fluids. Starting with pure or pseudo-pure components, empirical correlations for a NaCl brine and 1-hexadecene are taken from the literature. The library is implemented in Python 2.7 for use in a server powering simulation apps used by a large oil industry player, and engineers can request the generation of property tables for use in simulation software via a web app. The code was developed by researchers from our group, and commercial and open-source programs are used only for validation before releasing new versions. Preliminary results are verified against in-house experimental measurements of thermal conductivity, specific heat and density, and we propose adjustments to the available mixing rules.

Keywords: thermophysical properties, drilling fluids, mixture thermodynamics, computational library, Python 2.7

Introduction

After the construction of a well, the fluids using during the drilling stages become confined in the annular spaces between casing and tubing, interacting thermally with the production fluid and the surrounding rock formation (ALVES e BARBOSA JR., 2023). In various tasks related to wellbore design, engineers need to evaluate thermophysical properties of these fluids as a function of temperature and pressure.

There are several examples of computational libraries for evaluating thermophysical properties of fluids with high accuracy. REFPROP (MCLINDEN, 2018) is commercialized by the USA National Institute of Standards and Technology, while CoolProp (BELL, WRONSKI, *et al.*, 2014) is an open-source, freely available library that has wrappers in many programming languages. CoolProp has an extensive pure fluid library, although lacking some relevant components such as 1-hexadecene. CoolProp is relatively limited in terms of fluid mixtures.

The WelboreProps library developed by our group solves this problem by allowing the calculation of different properties for different fluids. The package is implemented in the Python language, version 2.7, for use in a legacy server that hosts a web app, of which WellboreProps is a component. When engineers request a wellbore simulation in the web app, they specify the fluids for each annular and the intended parameters, and the applications calls the library to generate the required tables for use of the simulation software.

In this work, we present the models used for the individual components of common drilling fluids, together with results for generated curves for selected properties and comparison with experimental data.

Numerical modeling of thermodynamic properties of pure fluids

The aqueous phase of brines is composed of NaCl brines, which are treated as a pseudo-pure component. This is valid as long as there is no precipitation of salt, i.e., the composition of the salt-water mixture is fixed, and the only variation is the proportion of the brine with relation with other components; the assumption of no interaction between the other components individually with salt or water is also necessary.

The volumetric basis for all brine calculations is the polynomial correlation developed by Zamora *et al.* (2013) for the density as a function of temperature and pressure. This correlation was developed for a single proportion (20% of salt in mass); this work assumes that this correlation can be linearly scaled for other salinity values.

For the volumetric properties of 1-hexadecene, a bi-quadratic polynomial (for temperature and pressure) was produced using values generated by Multiflash (INFOCHEM, 2014) with the Peng-Robinson equation applied. When data was not available, 1-hexadecene properties were considered equivalent to Diesel oil, using a composition presented by Martins, da Silva *et al.* (2022).

Table 1 shows the sources for individual properties correlations.

Table 1 - Sources for implemented correlations for pure or pseudo-pure components

Fluid	Density	Specific heat	Viscosity	Conductivity
NaCl Brine	(ZAMORA, ROY, *et al.*, 2013)	(CHEN, 1982)	(KESTIN e SHANKLAND, 1984)	(RAMIRES e CASTRO, 1994)
1-hexadecene	(KHASANSHIN, PODDUBSKI, *et al.*, 2006)	(KHASANSHIN, PODDUBSKI, *et al.*, 2006)	(INFOCHEM, 2014)	(YAWS, 1995)

Source: The authors

Experimental measurement of thermodynamic properties of pure fluids

To measure the thermal conductivity and volumetric specific heat, a commercial Guarded Hot Plate meter was used. This device was previously used in Alves, Czubinski, *et al.* (2022) to measure the thermal conductivity of paraffin-based fluid. The thermal conductivity is measured by applying a constant temperature difference to a sample of know thickness. By measuring the heat flow associated with the temperature difference, one determines the thermal conductivity via Fourier's law. In order to calibrate the heat flux sensor, the device is periodically verified against a standard Pyrex 7740 sample of known thermal conductivity, in a process which also determines the thermal contact resistance. The device measures the volumetric specific heat by imposing a constant temperature to the sample; after a stable condition is reached, the temperature is raised to a next set point, the cumulative heat flux necessary to change the temperature is measured and integrated in order to obtain the total heat.

The isobaric specific heat was measured using the MicroCalvet microcalorimeter from Setaram (SETARAM KEP TECHNOLOGIES, 2020). This calorimeter employs the Differential Scanning Calorimetry (DSC) method to measure the difference in heat capacity between two cells measured simultaneously. This procedure is better described in a companion paper (ALVES, DE CUNHA, *et al.*, 2024). The uncertainty of the experiment was computed using the deviation between the two calibration fluids and is determined to be within 3%.

The density was measured using a U-shaped vibrating-tube densimeter (Anton Paar, DMA-HPM). This type of instrument measures density based on the evaluation of the vibrating period of a hollow resonating tube filled with the sample fluid. The period depends on the temperature and pressure of the fluid. The DMA-HPM consists of a measurement cell and an interface module that measures the oscillation period and temperature of the tube containing the sample fluid. The density can be related to the oscillation period, temperature and pressure using a mathematical model (MAY, TAY, *et al.*, 2014) with adjustable parameters obtained through a calibration procedure using fluids with known densities.

Results and discussion

Figure 1 shows a comparison between calculated (with WellboreProps) and measured values for the specific heat of 1-hexadecene. The maximum deviation is of 9.45% relative to the measured values. The pressure is maintained in near atmospheric condition. The model predicts the experimental behavior with good accuracy, especially at lower temperatures; at higher temperatures, given that the model shows a continuous trend, there may be issues with the experimental procedure which must be repeated in the future to correct for any potential problems during measurement.

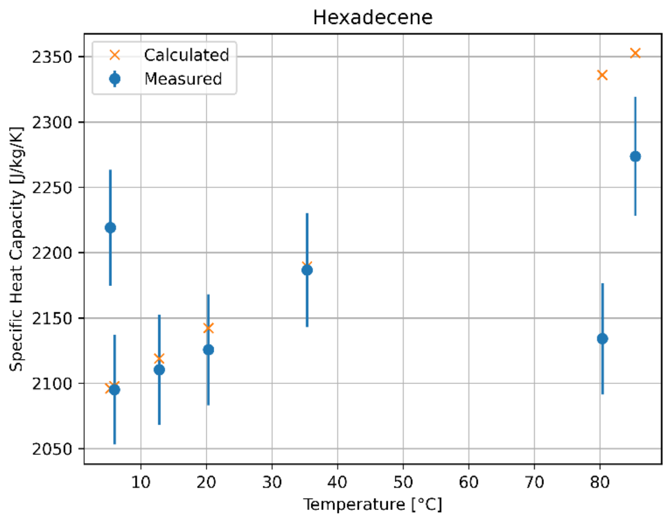

Figure 1 - Specific heat of 1-hexadecene

A dedicated measurement of just the density of 1-hexadecene is shown in Figure 2, where the overall trend is well-predicted but with a systematic deviation between model and measurement. The most likely explanation is the presence of contaminants in the 1-hexadecene sample, which makes the equation of state invalid.

Results for the conductivity of a NaCl brine with 12%-wt of mass fraction of salt (equivalent to a standard density of 9.06 ppg, which is what is used in WellboreProps) are shown in Figure 3. Despite the deviations below 6.11% being still larger than the experimental uncertainty, the trend is well predicted.

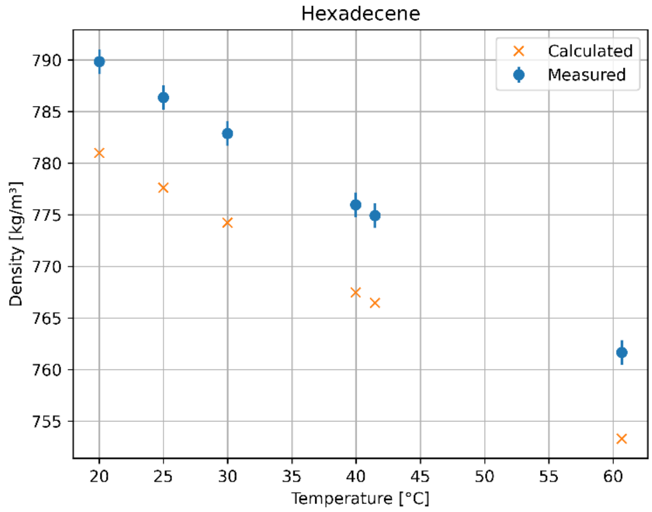

Figure 2 - Density of 1-hexadecene

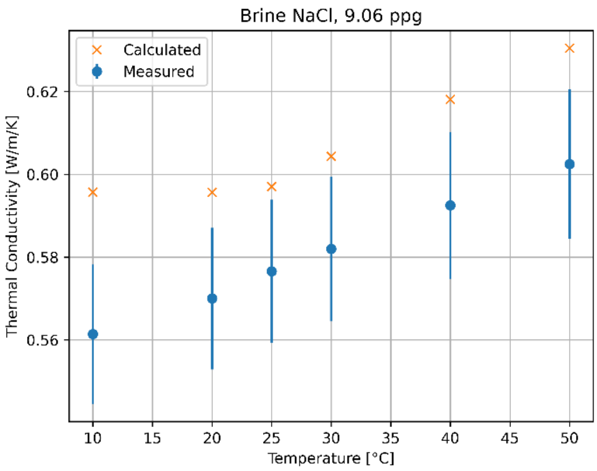

Figure 3 – Thermal conductivity of a NaCl Brine with 12%-wt of salt mass fraction

Conclusions

A computational library for the evaluation of thermophysical properties of drilling fluids is under development. Preliminary results for the pure and pseudo-pure components were shown in the present work, where the models for the density, specific heat and thermal conductivity of pure 1-hexadecene and one composition of a NaCl brine can predict experimental results under atmospheric pressure with deviations lower than 20%. Future works with expand the experimental database and propose new correlations for the afore-mentioned properties, in addition to measuring and modeling mixing rules for drilling fluids.

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