Fuel Doppler Coefficient of Reactivity in Highly Enriched Uranium-Fueled MSRs

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INTRODUCTION

The Doppler coefficient of reactivity of the nuclear fuel characterizes the change of core reactivity with fuel temperature before the fuel material can thermally expand. The term Doppler originates from the temperature-dependent Doppler broadening of resonances in the neutron cross-sections of the absorber, typically the ^{238}U part of the uranium fuel. The Doppler feedback is therefore the instantaneous component of the fuel temperature coefficient of reactivity (FTC). Hence, reactor designers prefer negative fuel Doppler feedback for safety reasons.

The Molten Chloride Reactor Experiment (MCRE) is a novel liquid-fueled fast-spectrum molten salt reactor (MSR) to be built at Idaho National Laboratory (INL) by TerraPower. Terrapower published [1] to establish a prototypical reference design to *support the development of modeling and simulation tools external to TerraPower*. As noted in this reference, the MCRE utilizes high-assay highly enriched uranium (HAHEU)[1] of 93.2% enrichment.

As the uranium enrichment increases in a fast-spectrum reactor, there are fewer resonance absorptions that result in neutron capture (n,γ) and more absorptions that result in fission, which makes the fuel Doppler reactivity coefficient (FDC) less negative. The analysis presented in this paper shows that MCRE, as defined in Reference [1], does not have a confidently negative FDC. However, the FTC contains the thermal expansion component and therefore is likely significantly negative. All scripts, analysis inputs, and plots relevant to this work are available on GitHub [2].

METHODOLOGY

This analysis models a slightly simplified version of MCRE, approximating the vessel as a 190-cm tall cylinder that is 100-cm in diameter, surrounded by 2-cm thick layer of magnesium oxide (MgO) reflector [1]. The fuel is a NaCl-UCl_3 (66.7-33.3 mol%) mixture of 93% enriched uranium and 99.9% enriched chlorine, with a mass density of 3.164 g/cm^3. The temperature of the fuel is changed, keeping all other model parameters constant. The core reactivity dependence on fuel temperature is fitted by a linear function, the slope of which is the FDC. The error of the FDC is found as a square root of the corresponding diagonal element of the covariance matrix of the least-square fit, also known as the asymptotic standard error of a fit parameter. Stochastic errors of MC transport runs are accounted for in the FDC fits, though it makes little difference since all the runs have the same statistics.

This paper presents results generated by SCALE/KENO-VI code version 6.3.1 [3] and reproduced by Serpent-2 [4]. Each run simulates 200,000 neutrons per generation in 2,510 total generations and 10 generations skipped. This large number of active histories, 5×10^8 for each run, is justified by the desire to lower the stochastic error since the effect is small. All simulation runs were performed at the high-performance computing cluster of the University of Tennessee at Knoxville, Department of Nuclear Engineering. Each run took about 40 minutes on a 64-core machine.

[1]HAHEU refers to uranium enriched above 80% in the ^{235}U isotope.

RESULTS

Nominal Model with 93% Enrichment

The baseline concept was analyzed in the temperature range from 500°C to 700°C in 21 steps of 10 K. The results are shown in Figures 1 and 2 for the ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data libraries, respectively. The results are supported by similar findings using Serpent-2, as shown in Figures 3 and 4. As noted in the plot, the FDC was calculated to be 0.015 pcm/K with a standard deviation of 0.014 pcm/K. These figures indicate the FDC is nearly zero for the MCRE-like concept and, when accounting for nuclear data and stochastic uncertainty, are almost certainly not guaranteed to be confidently negative. To further explore the impact of stochastic error, additional calculations were performed with significantly higher statistics.

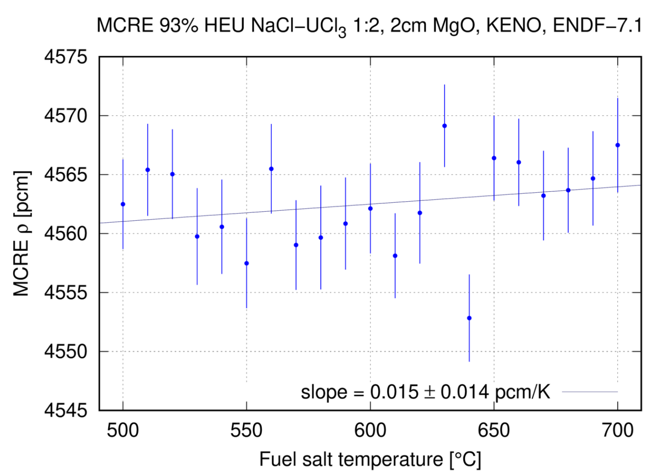

Fig. 1. MCRE reactivity vs. fuel temperature, ENDF/B-VII.I.

High-Statistics Runs at Two Temperatures

Uncertainty of a Monte-Carlo transport calculation can be arbitrarily reduced by a quadratically increased number of histories. The high-statistics runs feature 2,000,000 histories per generation, 25,020 total generations with 20 skipped; 5×10^{10} active histories in total. Only two temperatures are simulated,

TABLE I. Change in k_{eff} due to FDC, results from high-statistics simulations.

Nuclear Data Library	k_{eff} at 550°C	k_{eff} at 650°C	Δk_{eff} [pcm]
ENDF/B-VII.I	1.0477894 ± 0.0000038	1.0478015 ± 0.0000038	1.210 ± 0.537
ENDF/B-VIII.0	1.0472751 ± 0.0000040	1.0472925 ± 0.0000038	1.740 ± 0.552

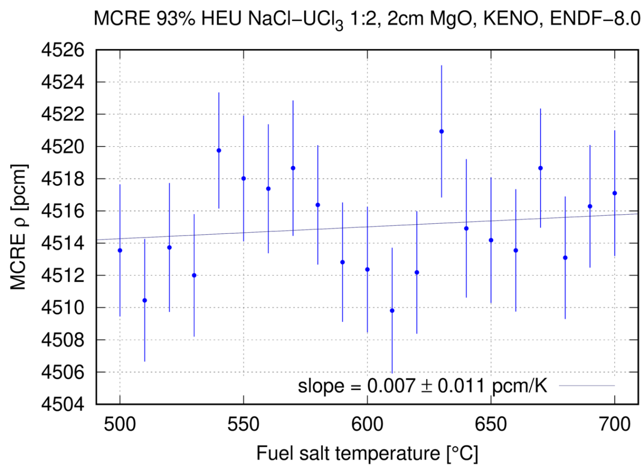

Fig. 2. MCRE reactivity vs. fuel temperature, ENDF/B-VIII.0.

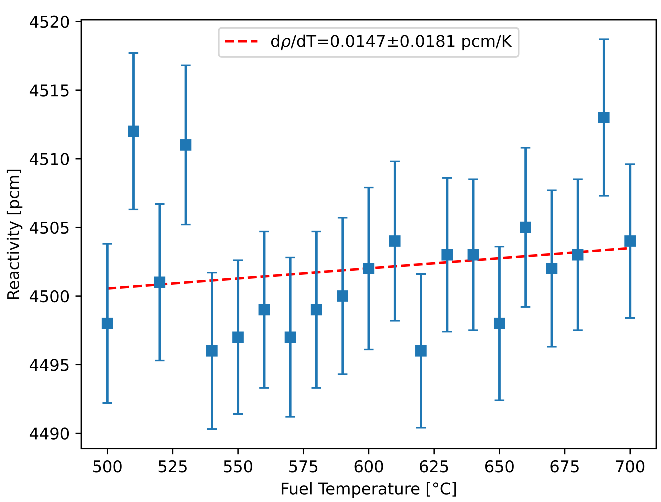

Fig. 3. MCRE reactivity vs. fuel temperature, ENDF/B-VII.I, Serpent-2.

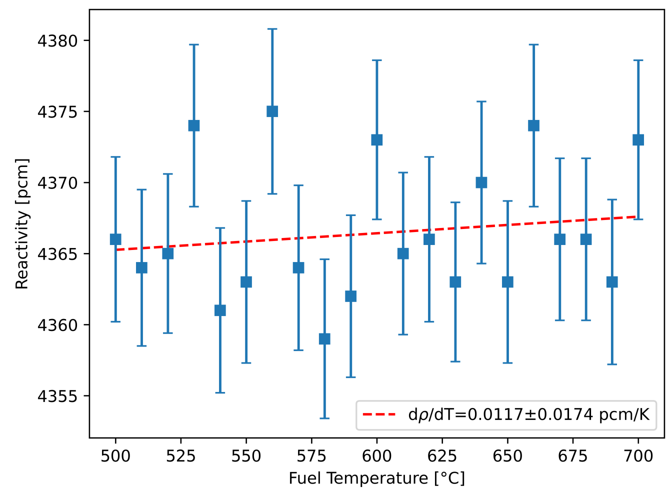

Fig. 4. MCRE reactivity vs. fuel temperature, ENDF/B-VIII.0, Serpent-2.

550°C and 650°C; results are shown in Table I using two different nuclear data libraries (ENDF/B-VII.1 and VIII.0). The difference in k_{eff} due to the fuel Doppler feedback for this 100°C change is shown. The results with improved statistics indicate that the FDC is positive (0.0121 to 0.0174 pcm/K) with more than two standard deviations (0.0054 to 0.0057). This further supports the findings that the MCRE concept, as modeled in this study, may have a slightly positive Doppler coefficient of reactivity.

FDC Dependency on Fuel Enrichment

To elucidate that this is closely related to the fuel enrichment, a suite of hypothetical MCRE-like core are modeled with fuel-bearing uranium enriched between 20% and 95%. For each value of fuel enrichment, a critical core dimension was found by scaling MCRE's linear dimensions. The critical diameter, D, and height, H, found for each enrichment value is shown in Table II.

For each enrichment value, the same simulations are performed to find the FDC as in the baseline case, using ENDF/B-VII.I nuclear data. Results for 20% and 45% enriched uranium cases are shown in Figures 5 and 6 respectively. The first figure indicates that the resonance absorption on 20% enriched uranium leads to a significantly negative Doppler feedback, while the 45% enriched fuel shows a weekly positive FDC.

The overall trend of fuel Doppler reactivity coefficient dependency on uranium enrichment is visualized in Figure 7. The blue diamonds indicate the FDC values, and the shaded band corresponds to errors of the parameter fits. The absolute value of FDC decreases quickly from 20% to 35% enrichment. With further increased enrichment, the FDC stays close to

TABLE II. Generic MCRE critical dimensions vs. enrichment.

U Enrichment [%]	D [cm]	H [cm]
20.0	258.883	491.877
25.0	215.916	410.240
30.0	189.297	359.664
35.0	170.716	324.361
40.0	156.837	297.991
45.0	145.790	277.002
50.0	136.687	259.705
55.0	129.023	245.144
60.0	122.513	232.774
65.0	116.794	221.909
70.0	111.777	212.376
75.0	107.293	203.857
80.0	103.273	196.219
85.0	99.644	189.323
90.0	96.348	183.062
95.0	93.310	177.289

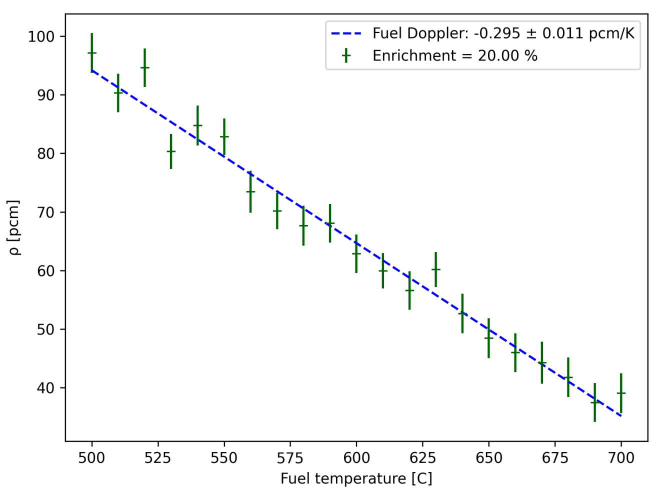

Fig. 5. Reactivity vs. fuel temperature for 20% enriched core.

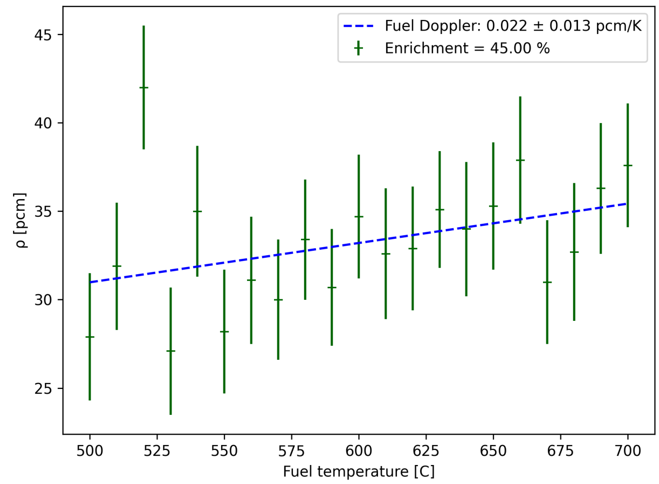

Fig. 6. Reactivity vs. fuel temperature for 45% enriched core.

zero, but mostly positive, though for each enrichment value its significance is near or within one standard deviation.

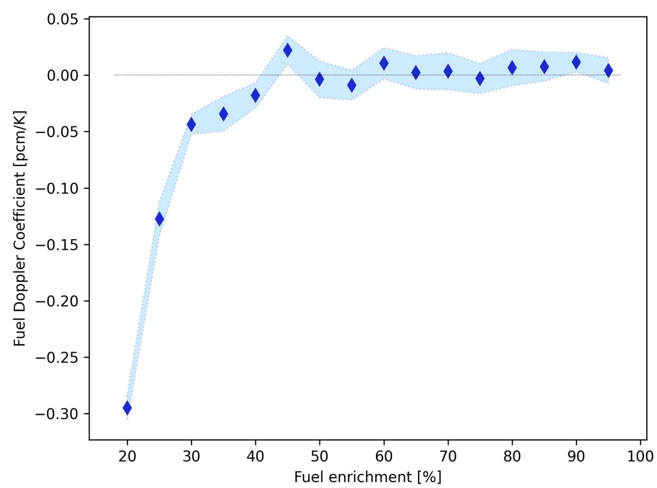

Fig. 7. FDC as a function of uranium enrichment.

DISCUSSION

The negative Doppler feedback coefficient of reactor fuel depends on a sufficient concentration of a resonant absorber, such as ^{238}U. With increasing fuel enrichment and hardening of the spectrum, the FDC weakens as more resonance absorptions result in fissions and fewer in parasitic capture, and may become positive. A positive FDC may lead to a burst-like dynamic behavior seen in the Godiva experiment [5, 6], where the power increases with temperature until the core expands thermally and the increased leakage reduces reactivity to below critical. Unlike Godiva, the MCRE is not a bare, solid-fueled reactor, but the fuel volume in the core is bound by the surrounding vessel. When heated, the fuel will expand and reduce the fissile mass in the core; however, the timescale upon which this happens must be considered.

During a power pulse, the fuel salt will heat and thermally expand through a pressure wave that will reach the reactor core vessel, including inlet and outlet piping. MCRE's neutron mean-free path is about 8 cm and the generation time about 0.1 μs, indicating a speed of neutron field propagation of about 800 km/s (80 cm/μs). This is much larger than the speed of sound in the fuel salt (about 1 km/s if there are no gases[2]). Because the neutron speed is greater than the speed of sound in the liquid, the power can increase throughout the reactor before the thermal expansion at the center can push salt mass out of the core. With a slightly positive Doppler coefficient, the power and temperature could potentially increase significantly before the core fissile mass is reduced to create a subcritical state. If the Doppler coefficient is slightly positive, a small reactivity increase could potentially lead to a prompt critical situation, like in the Godiva burst experiments. For comparison, the neutron propagation speed in a thermal MSR is only about 0.1 km/s (0.01 cm/μs), which is much less than the speed of sound in the liquid.

In a followup study, we noticed that increasing the MgO reflector thickness to 2 meters on all sides lowers the FDC to -0.05 pcm/K (the temperature of the reflector does not change). This value is still not considered confidently negative, given the potential influence of uncertainties in neutron cross-sections and the influence of absorptive impurities.

Lastly, Monte-Carlo transport codes such as SCALE/KENO and Serpent are not ideal tools for this problem. The statistical errors in the simulations presented are too large; however, cross-section uncertainties in the fast spectrum may be comparable to the stochastic errors in these runs. Uncertainty quantification is beyond the scope of this exercise. Assessing the safety of a HAHEU-fueled reactor should be done in a suitable radiation-hydrodynamic multiphysics framework, where the impulse transfer between the fuel and the surrounding vessel can be quantified. This short paper is intended to indicate the need for such analysis, not to provide final answers.

CONCLUSIONS AND FUTURE WORK

This work demonstrates that a generic MCRE-like concept does not have a confidently negative fuel Doppler coefficient of reactivity due to high ^{235}U enrichment. Further investigation into the safety implications of MCRE's Doppler coefficient and liquid fuel is needed. Because of the time delay between neutron field propagation (fuel Doppler feedback) and fuel salt thermal expansion (fuel density feedback), a prompt critical state may occur in response to a reactivity insertion event. The large amount of energy released during prompt criticality with a faster-than-sound neutron field propagation may exert significant pressure on the reactor vessel and raise structural integrity concerns.

Future modeling work is encouraged with sophisticated tools that allow for multiphysics coupling capable of capturing the neutron field propagation and impulses exerted on the reactor vessel. In addition, it would be of value to engage with the authors of Reference [1] to provide an updated reference design and materials that are less susceptible to this accident scenario.

The data and findings in this report are publicly available on GitHub [2]. We welcome researchers to take a look at our work and collaborate with us.

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REFERENCES

1. N. ULLAH, M. WARGON, K. WARDLE, M. BLATNIK, D. WALTER, T. CISNEROS, S. GOODRICH, and Z. MAUSOLFF, "MCRE-ENG-PRSNT-0029: MCRE Design Description in Support of External Model Development," Tech. rep., TerraPower (2023).
2. ONDREJ CHVALA, "Scripts, simulation input & output files, and plots relevant to this analysis ," `https://github.com/ondrejch/Doppler_HAHEU_MCFR/` (2024).
3. W. A. WIESELQUIST, R. A. LEFEBVRE, and M. A. JESSEE, "SCALE Code System," Tech. Rep. ORNL/TM-2005/39, Oak Ridge National Laboratory, Oak Ridge, TN (2020), version 6.3.1.
4. J. LEPPÄNEN, M. PUSA, T. VIITANEN, V. VALTAVIRTA, and T. KALTIAISENAHO, "The Serpent Monte Carlo code: Status, development and applications in 2013," *Annals of Nuclear Energy*, **82**, 142–150 (2015).
5. T. WIMETT, L. ENGLE, G. GRAVES, G. KEEPIN JR, and J. ORNDOFF, "Time behavior of Godiva through prompt critical," Tech. rep., Los Alamos Scientific Lab., N. Mex. (1956).
6. M. AUFIERO, C. FIORINA, A. LAUREAU, P. RUBIOLO, and V. VALTAVIRTA, "Serpent–OpenFOAM coupling in transient mode: simulation of a Godiva prompt critical burst," *Proceedings of M&C+ SNA+ MC*, pp. 19–23 (2015).

[2] The presence of gas voids, "bubbles," in a liquid makes the liquid compressible, and thus reduces its speed of sound.