

A DIGITAL TWIN-BASED SIMULATOR FOR SMALL MODULAR AND MICROREACTORS

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ABSTRACT

This paper reports preliminary work done on a mechanistic-based model digital twin (DT) for Gen IV reactors. The case study is a conceptual 4.5 MWth Small Modular Lead-cooled Fast (LFR) Research Reactor whose design incorporated aspects from all the three existing families of Gen IV LFRs. The back end for the DT exploited a modular approach consisting of the Neutronics and Thermohydraulic Coupling of the reactor core. This modular approach gives room for subsequent modification and/or addition of new blocks as the design concept matures without perturbing the entire system. After benchmarking simulation results with data from literature, the system's GUI demonstrated the capability to perform and visualize common operational transients either as a stand-alone simulator or in real-time using the MQTT broker. Insights derived from this virtual environment could contribute towards the ongoing refinement of LFR technology thus accelerating development through design testing, visualization, and optimization.

1 INTRODUCTION

The urgent need for zero-emission technologies, crucial to mitigating climate change and global warming, has sparked widespread interest in nuclear energy. It is recognized as a reliable and environmentally friendly energy source that does not emit greenhouse gases. In 2020, the International Atomic Energy Agency (IAEA) through the 14th Generation IV International Forum (GIF) made a call for faster deployment of Advanced (Next Generation or Generation IV (Gen IV)) Small Modular Reactor (SMR) and Micro Reactor (MR) Technologies. A number of these reactor technologies are currently being developed, some of which will be deployed before the end of this decade. It is important to mention that due to their; (i) – lower initial capital investment costs, (ii) – shorter construction times, (iii) – scalability and siting flexibility, (iv) – enhanced safety and (v) – small grid compatibility, SMRs and MRs are suited for a wide range of applications, spanning from industrial process heat generation to electrification of remote areas, small communities, and low-income countries.

But with novelty comes complexity. In other words, the technical know-how needed to build, operate, and maintain these reactors is still evolving – which is why advanced simulators or Digital Twin-based simulators present a unique opportunity for accelerated development through *design visualization*, *testing* and *system optimization*. Due to their inevitable role in Industry 4.0, coupled with recent advances on the Internet of Things (IoT), Digital Twin (DT)-based technologies have permeated almost every engineering discipline. As Kochunas notes in his review article on DTs for nuclear power applications, industries that do not successfully transition through this phase will likely be diminished. The United States Nuclear Regulatory Commission (U.S.NRC) defines a digital twin (DT) as *a virtual representation of an entity, process, or system, synchronized at a frequency and fidelity sufficient to maintain state concurrence. DTs leverage various types of models, data, and frameworks to produce insights about the represented entity, process, or system to fulfil an intended purpose*. This definition thus incorporates both physical assets and conceptual designs like the Gen IV Reactors. DTs for nuclear reactors (NRs) have been reported in the literature, some of which have integrated physics and/or AI/ML-based techniques to either detect system

faults or predict the reactor's evolution as summarized here (Liu et al. 2024). Kochunas recommends that DTs for NRs should first rely on *mechanistic model-based methods* to leverage the extensive experience and understanding of these systems, while, *model-free (AI or data-driven) techniques* can then be adopted to selectively, and correctively, augment limitations in the model-based approaches (Kochunas and Huan 2021). This paper, therefore, describes preliminary work done on a mechanistic/physics-based model DT for Gen IV reactors.

The case study is a **4.5 MWth Small Modular Research Lead-cooled Fast Reactor (LFR)**. *It is an ultra-safe research reactor that was conceptualized and designed from scratch during a group class project, at Texas A&M University (TAMU), Department of Nuclear Engineering.* It is worth noting that this reactor incorporated aspects from all three families of Gen IV LFRs. The motivation had been to design a *pool-type* 4.5 MWth LFR which could be directly installed at the TAMU's Nuclear Engineering Science Center (NESC) to work in tandem with the existing 1 MWth TRIGA reactor, with minimal or little modifications on the existing building. That is, the neutron source (*that serves for initiating the fission chain reaction during start-up*) would be removed from the TRIGA core, making it a sub-critical assembly (i.e. it cannot sustain a nuclear chain reaction on its own). The fast neutrons coming from the LFR's core will then activate and drive the TRIGA, generating a thermal neutron flux, hence the so-called **Fast and Thermal (FAT) Neutron Spectra Research Reactor**. These fast and thermal neutron fluxes from the LFR and TRIGA respectively could create new research and isotope production capabilities.

Since the TRIGA reactor already exists, most of the effort was directed towards the design of the 4.5 MWth LFR. While the Monte Carlo Simulations for neutron flux determination and burn-up calculations using MCNP have been dedicated as a topic of another research paper, this paper reports preliminary work done in modelling the dynamics of FAT's LFR core using SIMULINK/MATLAB and continuous efforts made so far (as a proof of concept) to build a DT-based simulator that enables real-time monitoring and prediction of the reactor's **thermal power, temperature transients**, and other parameters of interest, while receiving real-time data as inputs. It is envisaged that continued development of the FAT research reactor and this associated DT will occur in tandem, with the DT leveraging opportunities for risk-free experimentation, monitoring, and data analysis, which will provide feedback for the refinement of FAT's concepts.

For the remainder of this paper, a brief description of the conceptual design of FAT's 4.5 MWth LFR is given in section 2, followed by a detailed description of the backend development and the associated DT architecture. The results are presented in section 3, with the conclusion and remarks for future development given in section 4.

2 MATERIALS AND METHODS

As mentioned earlier, the case study for this DT-based simulator is a conceptual 4.5 MWth LFR. Stability and safety analyses performed on this reactor (reported in this study) have suggested a compact, ultra-safe system since we fused peculiarities from all the three existing LFR families shown in Figure 1. SIMULINK and MATLAB's App Designer both presented capabilities to modularly solve and visualize reactor transients, and add new modules without perturbing the system performance, thus conforming to the overall goals of the FAT project. Particularly, the **Message Queuing Telemetry Transport (MQTT)**, a lightweight, publish-subscribe, machine-to-machine network protocol of the **Internet of Things (IoT)**, was exploited to achieve real-time data transfer and visualization of operating transients as discussed in detail in section 3.5.

2.1 Conceptual Design and Brief Description of Lead-cooled Fast Reactors (LFRs)

The LFR is one of six reactor technologies selected by GIF as candidates for advanced (Gen IV) reactors. In brief, it is a **fast neutron spectrum reactor** that uses liquid metal (lead (Pb) or lead-bismuth eutectic (LBE)) as its primary coolant. Three reference systems currently exist namely, the European Lead-cooled Fast Reactor (ELFR), the Russian BREST, and the United States' Small Secure Transportable Autonomous Reactor (SSTAR). Though they share common safety features, significant material and structural

differences exist as shown in Figure 1. Details about these can be found in dedicated literature (Alemberti, et al. 2020; Alemberti et al. 2014; Alemberti, et al. 2020). ALRED stands for Advanced Lead-cooled Fast Reactor European Demonstrator. It is a scaled-down version aimed to demonstrate the viability of the ELFR technology for future commercial power plants.

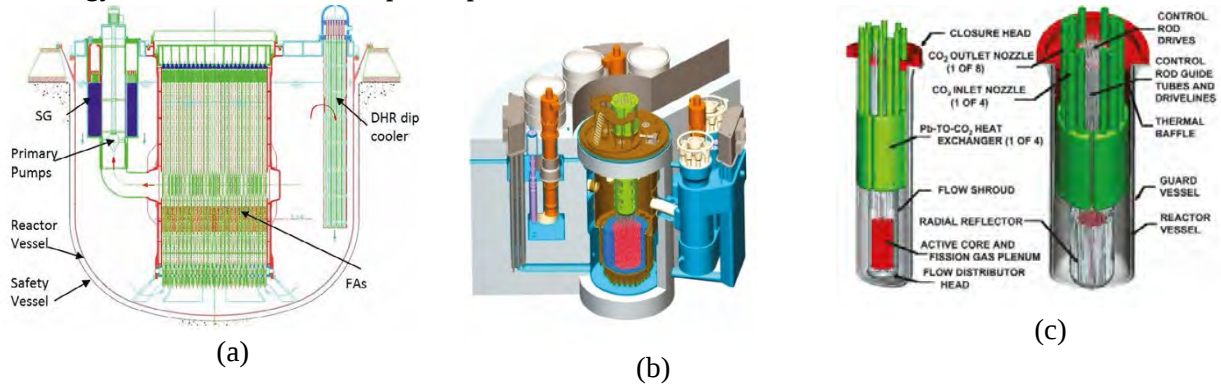


Figure 1: Generation IV International Forum (GIF) – LFRS reference systems (GIF Annual Report 2022); (a)- ELFR, (b)- BREST and (c)- SSTAR (definitions given in the text). These are presented to give an idea of what features were adapted for our 4.5 MWth LFR, like the structural similarity with ELFR which is elaborated in the text.

Also elaborated in Table 1 are the main design parameters of these reactors, presented here to highlight features that were adapted for our 4.5 MWth LFR, like the lead (Pb) coolant from ELFR, ALFRED and SSTAR and EP823 cladding from BREST.

Table 1: Main parameters of reviewed LFR designs. Note that FAT is 4.5 MWth which is a scaled-down SSTAR by a factor of 10.

LFR Family	Power [MWth]	Cladding	Core inlet T [°C]	Core outlet T [°C]	Coolant type/Velocity [m/s]
ELFR	1500	T91	400	480	Pb/1.6
ALFRED-125	300	15-15Ti	400	480	Pb/1.4
BREST-300	700	EP823	420	540	LBE/1.8
STAR	45	HT9	420	567	Pb/0.896

As shown in Figure 2, the base design of FAT's LFR consists of a hexagonal lattice with hexagonal fuel pins, based on SSTAR's compact design (scaling down by a factor of 10), while the material for the cladding – the EP823-Sh ferritic-martensitic steel was adopted from BREST. The EP823 was specifically developed to be used with lead-cooled systems due to its resistance to corrosion through the formation of a protective film (i.e. iron and chromium–based oxide layers) under controlled oxygen conditions and optimal flow velocities (Anderoglu et al., 2021; Zhang 2009). The main vessel (reactor module) then incorporated safety features from ALFRED. This consisted of; the **Inner Vessel (IV)** which holds the Fuel Assemblies (FAs), the **Reactor Vessel (RV)** which houses the inner vessel, the primary coolant, the downcomer (DC) and the **Safety Vessel (SV) or Guard vessel (GV)** housing both the RV and IV. The GV retains the coolant in case of any failures that might result in ruptures and leaks in the RV during operation. This ensures that natural circulation for heat removal is maintained while providing sufficient grace time for appropriate interventions. Lastly, Metal fuel was chosen for the core due to its inherent passive safety and superior conductivity when compared to mixed oxide (MOX) fuels as detailed here (Fast Reactor Working Group 2018). **These design selections culminated in an ultra-safe 4.5 MWth research reactor.** The next session focuses on the dynamics of the reactor core which is currently the backbone of this digital twin.

2.2 Back-end Development of the DT: NTC Coupling

This incorporated a modular physics-based approach consisting of the **Neutronics – Thermohydraulic Coupling** (hereafter referred to as NTC) of the reactor core. Note that the *neutronics* (neutronic module) describes the time rate of heat (power) **generated** via nuclear fission of the nuclear fuel. This process can be described by the so-called Point Reactor Kinetics Equations (PRKEs), which is a reduced order (**zero-dimensional**) set of ordinary differential equations (ODEs). The thermal hydraulics (thermohydraulic) module on the other hand describes the time rate of heat (power) **transferred** from the fuel rods through the cladding into the coolant (in this case liquid lead) via a set of energy balance ODEs. Focus was laid on average values (temperature and power), hence the so-called **lumped parameter** approach. These two modules are coupled together through a reactivity feedback loop for temperature and an input loop for control rods and mass flow (see Figure 2). This modular approach gives room for subsequent modification and/or addition of new blocks as the design concept matures without perturbing the whole system.

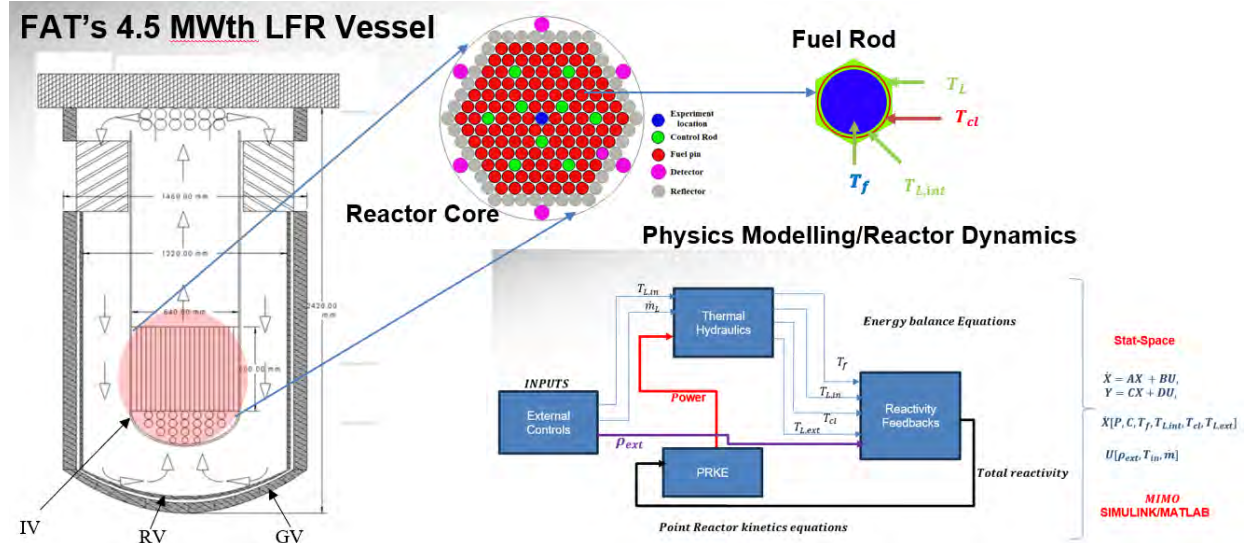


Figure 2: FAT's 4.5 MWth Reactor conceptual design, detailing the reactor core and schematic representation of the NTC coupling (blue rectangles).

Note that similar NTC approaches have been reported in the literature, mostly studying the dynamics of ALFRED, the only LFR reactor publicly available for data sourcing (Colombo et al. 2010; Lorenzi, Cammi, et al. 2013; Shahzad et al. 2018). This paper however presents novelty not only in terms of application field but also in terms of the design of experiments. Our GUI serves as an interface for physics-based Digital Twins interpretation, extending the capabilities of such traditional simulators to incorporate real-time visualizations for new reactor concepts. This outlines the relevance of DTs for critical systems such as nuclear energy, nuclear propulsion systems, aerospace, and others. These kinds of use cases help the community to grow in visibility and knowledge about the needs of critical systems to be developed. For brevity, all parameters used in the model have been summarized in Table 2.

Table 2: Nomenclature of parameters of the Physics-based Point Reactor Kinetics Equations (PRKEs describing fission) and the Thermohydraulic (Energy) balance equations describing the heat transfer.

Quantity	Meaning [units]	Quantity	Meaning [units]
P_0	Nominal Power [Wth]	h_{Lcl}	Lead-cladding overall heat transfer coefficient [WK^{-1}]
Λ	Average neutron lifetime [s]	M_{cl}	Mass of cladding

Quantity	Meaning [units]	Quantity	Meaning [units]
β	Delayed neutron fraction [pcm] at BOC	C_{cl}	Specific heat capacity of cladding at constant pressure [$J kg^{-1}K^{-1}$]
β_i	i^{th} precursor group delayed neutron fraction (pcm)	h_L	Cladding-coolant overall heat transfer coefficient [WK^{-1}]
λ_i	i^{th} precursor decay constant [s^{-1}]	M_L	Mass of coolant [kg]
α_D	Doppler Effect coefficient of reactivity [$pcm K^{-1}$]	$\dot{m}_L$	Coolant flow rate of [$kg s^{-1}$]
α_z	Axial expansion coefficient of reactivity [$pcm K^{-1}$]	k_f	Thermal conductivity of Fuel [$W m^{-1}K^{-1}$]
α_r	Radial expansion coefficient of reactivity [$pcm K^{-1}$]	k_L	Thermal conductivity of lead [$W m^{-1}K^{-1}$]
α_L	coolant expansion coefficient of reactivity [$pcm K^{-1}$]	D_h	Hydraulic diameter of flow [cm]
α_H	Control rod worth coefficient of reactivity [$pcm cm^{-1}$]	Nu	Nusselt number
T_f	Fuel temperature[°C]	k_f	Thermal Conductivity of Fuel [W/m.K]
$T_{L,int}$	Internal lead temperature[°C]	r_f	Fuel pin outer radius [cm]
T_{cl}	Cladding temperature[°C]	r_L	lead column radius [cm]
T_L	Coolant temperature[°C]	r_{cl}	Cladding outer radius [cm]
T_{in}	Core inlet temperature [°C]	h_{fL}	Fuel-lead overall heat transfer coefficient [WK^{-1}]
T_{out}	Core outlet temperature [°C]	$M_{L,int}$	Mass of internal lead [kg]
M_f	Mass of fuel meat [kg]	C_L	Specific heat capacity of lead at constant pressure [$J kg^{-1}K^{-1}$]
C_f	Specific heat capacity of fuel meat at constant pressure [$Jkg^{-1}K^{-1}$]	H_f	Active core height

So, the following **PRKEs**, based on the six-group delayed neutron precursors were used,

$$\begin{cases} \frac{dP(t)}{dt} = \frac{\rho - \beta}{\Lambda} P(t) - \sum_{i=1}^6 \lambda_i C_i(t) \\ \frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} P(t) - \lambda_i C_i(t), \quad i = 1, 2, \dots, 6 \end{cases} \quad (1)$$

Because of the peculiar design of the fuel pin, four different energy balance equations were derived for the thermal-hydraulics (TH) loop. That is,

$$\left\{ \begin{array}{l} M_f C_f \frac{dT_f}{dt} = P(t) - h_{fL}(T_f - T_{L,int}) \\ M_{L,int} C_L \frac{dT_{L,int}}{dt} = h_{fL}(T_f - T_{L,int}) - h_{Lcl}(T_{L,int} - T_{cl}) \\ M_{cl} C_{cl} \frac{dT_{cl}}{dt} = h_{Lcl}(T_{L,int} - T_{cl}) - h_L(T_{cl} - T_L) \\ M_L C_L \frac{dT_L}{dt} = h_L(T_{cl} - T_L) - 2\dot{m}_L C_L(T_L - T_{in}) \end{array} \right. \quad (2)$$

Note that the second relation in equation (2) is introduced to account for conduction through the lead-filled gap which is often neglected for fuel pins having a gas-filled gap. The bulk temperature of the coolant (T_L) was expressed as an average of the coolant inlet and outlet temperatures T_{in} and T_{out} respectively.

$$T_L = \frac{T_{out} + T_{in}}{2} \quad (3)$$

The associated heat transfer coefficients [WK^{-1}] were modified (Todreas and Kazimi, 2021) to fit this reactor design as follows.

$$\begin{aligned} h_{fL} &= \frac{1}{\frac{1}{4\pi H_f k_f} + \frac{\ln(r_L/r_f)}{2\pi H_f k_L}} \\ h_{Lcl} &= \frac{1}{\frac{\ln(r_{cl}/r_L)}{2\pi H_f k_{cl}}} \\ h_L &= \frac{1}{2\pi r_{cl} H_f h}, \text{ where } h = Nu \cdot \frac{k_L}{D_h} \end{aligned} \quad (4)$$

The total reactivity was also defined as follows.

$$\rho(t) = \sum_i \alpha_i \Delta T_i \quad (5)$$

where α_i represents the reactivity coefficients of the fuel, cladding, coolant, and control rods. Since metal fuel was used in this design, the values for α_i as well as delayed neutron yields and decay constants for the 6 groups of precursors at the beginning of the cycle (BOC) were adopted from ALFRED (Lorenzi, Ponciroli, et al. 2013). The above-coupled system of ODEs was then coded in SIMULINK/MATLAB, resulting in the simulator engine for the DT (not shown here for brevity). Simulation results and various operational transients were tested and benchmarked against existing data for ALRED as will be discussed in the proceeding sections.

3 RESULTS AND DISCUSSIONS

A series of design basis and operational transient experiments were performed to ascertain FAT's stability, safety, and functionality of this digital twin. This section reports findings obtained from both the SIMULINK environment and the system's GUI.

3.1 Sanity Checks of the Simulator Engine

To verify the reliability, accuracy and response of the design, the following sanity/benchmarking checks were performed; **Case 1**-Steady State Response $\{\rho_{ext}, \dot{m}, T_{in}\} = \{0 \text{ pcm}, 155 \text{ kgs}^{-1}, 400^\circ \text{C}\}$; **Case 2**-Step reactivity insertion (10 pcm) after 600 s; **Case 3**-Step increase in the inlet temperature by 10°C ; and **Case 4**-Step increase in the mass flow rate by 10%. The power and temperature remain constant throughout the steady state, while an impulse response was observed under step inputs for all parameters except the fuel temperature. This behavior is like the one reported for ALFRED in the literature and therefore served as a benchmark of our NTC model. For brevity, the plots have been omitted since they are similar to the ones that will be reported in section 3.4 of this text.

3.2 Sensitivity Analysis: Ramp Inputs

The following rates were introduced into the reactor after 600 s. (i) - a 1 pcm/s reactivity increase, (ii) - a 1 °C/s temperature rise, and (iii) - a 1 (kg/s)/s mass flow rate increase, individually coded on the graphs as **rho**, **T_{in}** and **M_{dot}** respectively. Figure 3 represents the results obtained. We found that the reactor is least sensitive to changes in mass flow rate. As such, the mass flow rate was not considered as an input for stability analysis (discussed in section 3.3). However, it was maintained as an integral part of the input in the DT. It is important to note that the above response qualitatively resembles that of ALFRAD reported in the literature (Lorenzi, Cammi, et al. 2013; Shahzad et al. 2018) for similar perturbations. There are, however, small differences attributed to the peculiarity of this reactor design.

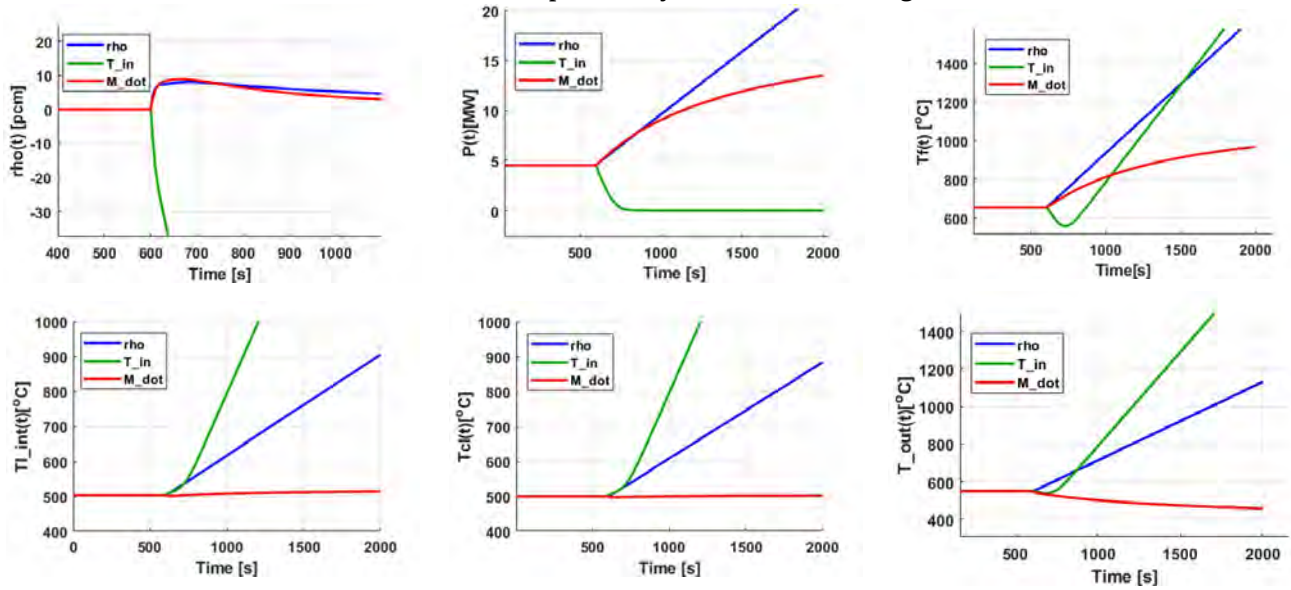


Figure 3: Reactor response from ramp inputs.

3.3 Stability Verification via the Pole-zero map

By examining the locations of poles and zeros of the transfer function in the complex plane, the stability of any dynamical system can be studied. The Lyapunov stability criterion states that *an open-loop linear time-invariant system such as our NTC model is stable if, in continuous time, all the poles of the transfer function lie in the left half of the complex s-plane. The system is marginally stable if distinct poles lie on the imaginary axis, that is, the real parts of the poles are zero* as shown in Figure 4 (a). Every system of ODEs can be represented in state space as follows.

$$\begin{cases} \dot{x}' = Ax + Bu \\ y = Cx + Du \end{cases} \quad (6)$$

For our NTC model, we defined $x = [P(t), C(t), T_f(t), T_{L_{int}}(t), T_{cl}(t), T_L(t)]^T$ as the vector of state variables and $u = [\rho_{ext}, T_{in}]^T$ to be the inputs. This resulted in the so-called **multiple input multiple output** model (**MIMO**), whose transfer function can be derived after determining the system matrices A, B, C and D (not given here for brevity). The two sets of Transfer functions, each set corresponding to a unit impulse excitation of the external reactivity (u_1) and the inlet temperature (u_2) were computed. We present the two sets of expressions for just the output power. Note that only the zeros (numerator) differ and therefore, similar expressions for the temperatures (not presented here) were also obtained.

$$G_1(s) = \frac{P(s)}{\rho_{ext}(s)} = \frac{6.541e12 s^5 + 2.886e15 s^4 + 8.034e16 s^3 + 2.128e17 s^2 + 3.018e16 s + 1.085e15}{s^6 + 5271 s^5 + 5.566e06 s^4 + 1.831e09 s^3 + 1.023e11 s^2 + 1.056e12 s + 8.694e10} \quad (7)$$

$$G_2(s) = \frac{P(s)}{T_{in}(s)} = \frac{-2.598e13 s^4 - 1.152e16 s^3 - 4.514e17 s^2 - 8.547e16 s - 3.991e15}{s^6 + 5271 s^5 + 5.566e06 s^4 + 1.831e09 s^3 + 1.023e11 s^2 + 1.056e12 s + 8.694e10} \quad (8)$$

The pole-zero maps for $G_2(s)$ represented in Figure 4 shows that our NTC model is stable.

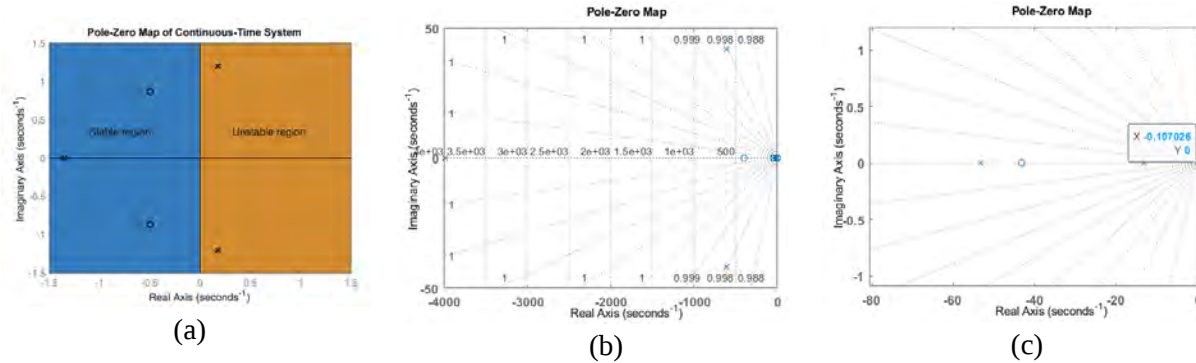


Figure 4: (a) - Stability criteria for dynamical systems taken from MATLAB 2022b documentation; (b) – Pole-zero map of FAT’s LFF’s Transfer function $G_2(s)$. Notice how all poles lie in the stability region or left half plane, suggesting that the reactor is stable; (c)- Zoomed plot showing the first pole.

Alternatively, the stability of a state space system can also be verified through **the eigenvalues of matrix A, which must All have negative real parts**. Our NTC reactor yielded the following results; $e_1 = -3988.7$, $e_2 = -607.67 + 41.80i$, $e_3 = -607.67 - 41.80i$, $e_4 = -53.2567$, $e_5 = -13.2900$, $e_6 = -0.0830$, further confirming stability.

3.4 Accidents (Deviations from normal operations) and SCRAM

The design peculiarities of this reactor just like the existing LFRs eliminate the possibility of loss of coolant accidents (LOCA) commonly observed with light water reactors. However, the following accident scenarios are common and were simulated; **UTOP** (Unprotected Transient of Overpower): This occurs when there is a malfunction of reactivity control of the system. A step reactivity of 20 pcm (0.0602 \$) was introduced at the input; **ULOHS** (Unprotected Loss of Heat Sink): This is the malfunction of the heat removal system of the FAT coolant (e.g., partial malfunction of one of the heat exchangers). Following a conservative approach, the inlet temperature of the coolant is increased by a 20 °C step; **ULOF** (Unprotected Loss of Flow): This is the malfunction in the natural circulation of the FAT coolant loop. This could be due to unexpected pressure variations in the primary or secondary.

SCRAM refers to an emergency shutdown of the reactor. A step reactivity of -15β , equivalent to $-4,984.1$ pcm (-15.0002 \$) was inserted into the core after 600 s. An impulsive response (Figure 5) of the power, reactivity, and temperatures (except the fuel temperature) as described earlier is observed. UTOP also seems to produce the least change in the system parameters as expected. Under the SCRAM scenario, shown in Figure 6, the reactor power rapidly decays to zero (as expected) while the temperatures all decrease to the coolant input value of 400 °C.

The convergence of two robust, alternative stability verifications as well as all the above operational transient verifications suggested that the FAT’s 4.5MWth LRR reactor with the present design parameters is very stable and can withstand extreme operating conditions and that this NTC model could serve as a starting point (input stage) for a DT for real-time implementation.

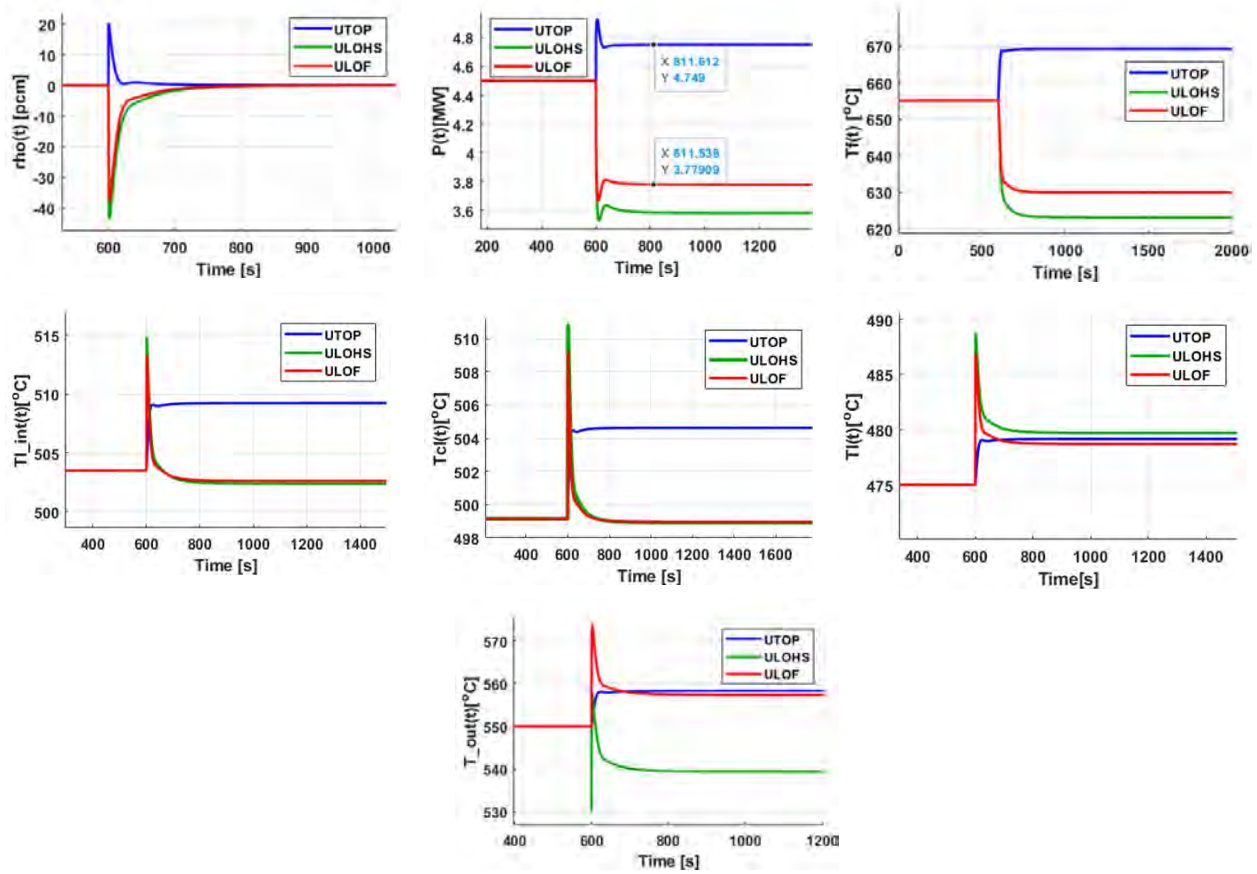


Figure 5: Reactor response to simulated accidents; UTOP, ULOHS and ULOF (definitions given in the text). Notice that the total reactivity always goes to zero at the new steady state, indicating stability.

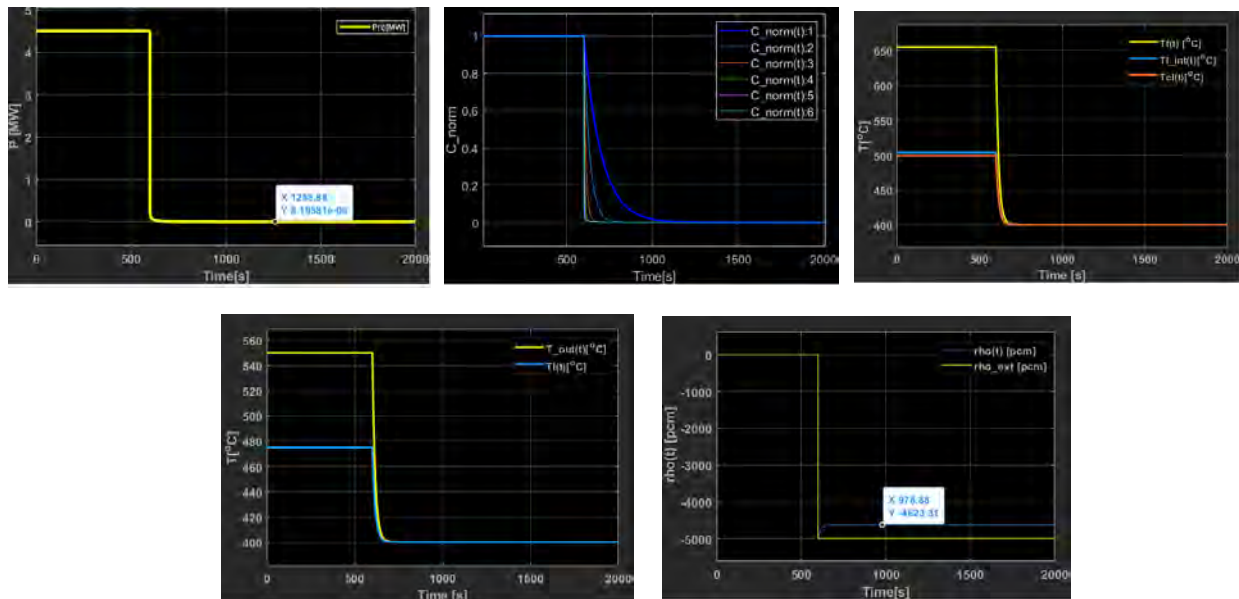


Figure 6: Reactor response to SCRAM; Power decays to zero and temperatures reduce to 400 °C.

3.5 Real-time Implementation and a GUI Interface

As mentioned earlier, the ability to visualize the system's evolution in real-time while making changes to it could be an invaluable tool for risk-free experimentation, design visualization, testing and optimization. MQTT as described in section 2, together with MATLAB's App designer and virtual sensors (Martin et al. 2021; Stavropoulos et al. 2023) were exploited to achieve this purpose since FAT is still a concept. Figure 7 shows the current version of this graphical user interface (GUI). It includes features that mimic a reactor's control room with our NTC SIMULINK model running in the background. Using the **ThingSpeak™** broker as the **virtual sensor platform**, we were able to mimic a real-time scenario by directly streaming recorded data from previous simulation runs as input to our channel and then reading these into the simulator.

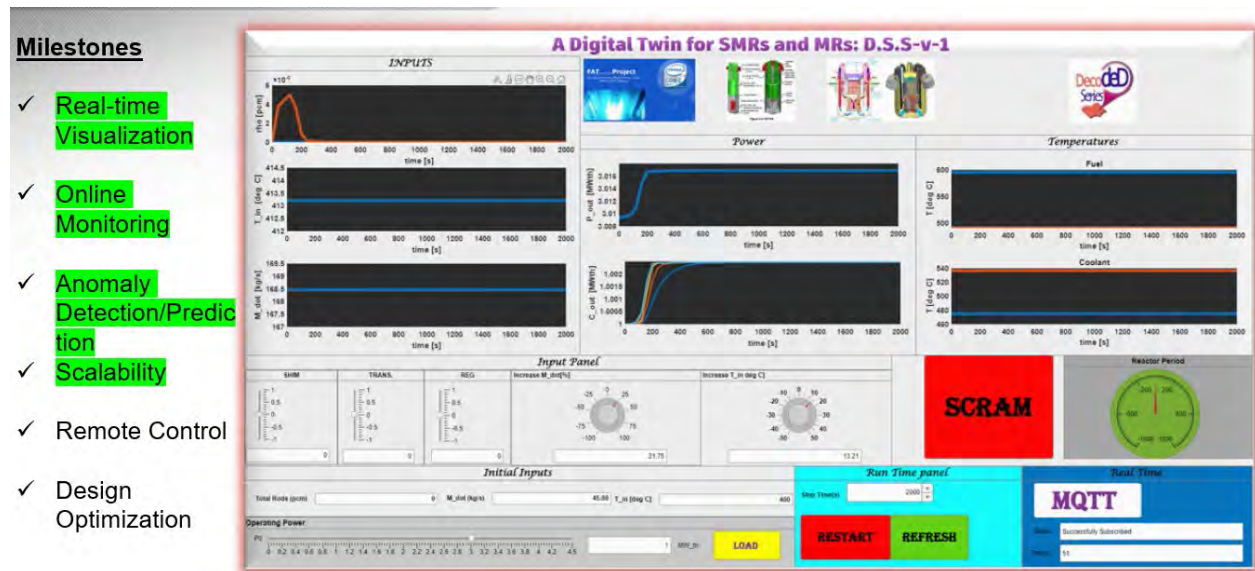


Figure 7: FAT's GUI demonstrating the reactor's response in real-time to a positive reactivity insertion. Notice the instantaneous change in outputs following the input changes.

Through this GUI, many operating transients were demonstrated as a stand-alone simulator together with real-time implementation. Through the Input Panel, changes in reactivity (by moving the control rods up/down), the mass flow rate or coolant temperature directly translate changes in the output reactor power and temperatures, visible on the dashboard. This function could enable the tool to be used for training. The real-time panel provides a seamless transition to real-time via access to the **ThingSpeak™** channel for loading real-time data (currently provided by virtual sensors) into the simulator.

4 CONCLUSION

This paper reported preliminary work done as proof of concept of a DT-based simulator for a 4.5 MWth LFR Gen IV reactor concept. A brief description of the rationale and the FAT reactor design was presented, followed by a detailed description of the DT's back-end development based on a scalable neutronic-thermal-hydraulics coupling model, and finally, the DT's front end with real-time implementation.

Results demonstrated the capability to perform and visualize common operational transients either as a stand-alone simulator or in real-time using the MQTT broker through the developed GUI. While this backend (NTC) model is currently being expanded to incorporate reactivity feedback from neutron poisons like xenon and samarium, its extension to predicting the power and temperature transients of the existing TRIGA reactor has already been achieved (not reported here for brevity). These findings so far suggest that the tool, when fully developed could be extended to incorporate other reactor systems. Future developments

like the integration of machine learning algorithms that will leverage historical and real-time data to enable predictive maintenance and anticipation of potential issues before they manifest are foreseen.

Also, comprehensive modelling could extend to the prediction of material behavior under various conditions, contributing to a holistic understanding of the reactor's performance. Therefore, it is envisaged that the insights derived from this virtual environment will contribute to the ongoing refinement of the LFR technology, thus fostering a more sustainable and secure energy future. Lastly, because the digital twin's core and Physics-based models can be easily adapted to fit any reactor technology and design (**by just modifying the parameters in Table 2**), *its usage, not only as a predictive but also a training tool for operators in reactor systems that will be deployed especially in the less developed countries where the technical know-how is currently limited cannot be overstated.*

REFERENCES

- Alemberti, A., M. Caramello, M. Frignani, G. Grasso, F. Merli, G. Morresi, and M. Tarantino. 2020. "ALFRED Reactor Coolant System Design". *Nuclear Engineering and Design*, 370. <https://doi.org/10.1016/j.nucengdes.2020.110884>.
- Alemberti, A., M. L. Frogheri, S. Hermesmeyer, L. Ammirabile, V. Smirnov, M. Takahashi *et al.* 2014. *Lead-cooled Fast Reactor (LFR) Risk and Safety Assessment White Paper*. https://gif.jaea.go.jp/methodology/rswg/rswg_lfr_white_paper_final_8.0.pdf.
- Alemberti, A., K. Tuček, M. Takahashi, T. Obara, M. Kondo, A. Moiseev *et al.* 2020. *Lead-cooled Fast Reactor System Safety Assessment Lead-cooled Fast Reactor (LFR) System Safety Assessment System Safety Assessment* https://gif.jaea.go.jp/methodology/rswg/gif_lfr_ssa_june_2020_2020-06-09_17-26-41_202.pdf.
- Anderoglu, O., A. Marino and P. Hosemann. 2021. "Corrosion in Heavy Liquid Metals for Energy Systems". *The Journal of The Minerals, Metals and Materials Society (TMS)* 73(12): 3998–3999. <https://doi.org/10.1007/s11837-021-04973-8>.
- Colombo, M., A. Cammi, V. Memoli, D. Papini, and M. E. Ricotti. 2010. "Transfer Function Modelling of the Lead-cooled Fast Reactor (LFR) Dynamics". *Progress in Nuclear Energy* 52(8): 715–729. <https://doi.org/10.1016/j.pnucene.2010.04.007>.
- Fast Reactor Working Group. 2018. *Fast Reactor Working Group - Nuclear Metal Fuel: Characteristics, Design, Manufacturing, Testing, and Operating History*. <https://www.nrc.gov/docs/ML1816/ML18165A249.pdf>.
- GIF Annual Report 2022. 2022. *GIF IV 2022 (Generation IV International Forum) Annual Report*. <https://www.gen-4.org/gif/>.
- Kochunas, B. and X. Huan. 2021. "Digital Twin Concepts with Uncertainty for Nuclear Power Applications". *Energies* 14(14). <https://doi.org/10.3390/en14144235>
- Liu, Y., F. Alsafadi, T. Mui, D. O'grady, and R. Hu. 2024. "Development of Whole System Digital Twins for Advanced Reactors: Leveraging Graph Neural Networks and SAM Simulations". *Nuclear Technologies*. In Press.
- Lorenzi, S., A. Cammi, S. Bortot, R. Ponciroli, and A. Moiseyev. 2013. "Analytical Models for a Small LFR Core Dynamics Studies". *Nuclear Engineering and Design*, 254: 67–88. <https://doi.org/10.1016/j.nucengdes.2012.09.001>.
- Lorenzi, S., R. Ponciroli, A. Cammi, and S. Bortot. 2013. "Development of a Control-oriented Simulator for a LFR Demonstrator". *Nuclear Engineering and Design*, 262: 319–339. <https://doi.org/10.1016/j.nucengdes.2013.04.027>.
- Martin, D., N. Kühl, and G. Satzger. 2021. "Virtual Sensors". *Business and Information Systems Engineering*, 63(3): 315–323. <https://doi.org/10.1007/s12599-021-00689-w>.
- Shahzad, M. A., L. Qin, and S. S. Imam. 2018. "Analysis of Lead-cooled Fast Reactor Using a Core Simulator". *Progress in Nuclear Energy*, 104: 229–241. <https://doi.org/10.1016/j.pnucene.2017.10.002>.
- Stavropoulos, G., J. Violos, S. Tsanakas, and A. Leivadreas. 2023. "Enabling Artificial Intelligent Virtual Sensors in an IoT Environment". *Sensors*, 23(3). <https://doi.org/10.3390/s23031328>.
- Todreas, N. E., and M. S. Kazimi. 2021. *Nuclear Systems I Thermal Hydraulic Fundamentals*. 3rd ed. Boca Raton. CRC Press.
- Zhang, J. 2009. "A Review of Steel Corrosion by Liquid Lead and Lead-bismuth". *Corrosion Science* 51(6): 1207–1227. <https://doi.org/10.1016/j.corsci.2009.03.013>.

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