# Simulating Circulating-Fuel Fast Reactors with the Coupled TRACE-PARCS Code

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**Abstract.** Fast reactors that circulate liquid fuel exhibit a strong coupling between neutronics and thermal-hydraulics (THs) that necessitates the use of coupled multi-physics codes to study dynamic behaviour. Presently, most such tools employ computational fluid dynamics (CFD) to resolve THs. This paper concerns an alternative approach in which the system code TRACE is used to compute two-dimensional flow patterns and temperature distributions of liquid-fuel fast reactors using coarse meshes and a simplified set of equations. As such, computational requirements are greatly reduced compared to CFD-based solvers. In the coupled tool, the TH variables are sent to the spatial neutronics solver PARCS that calculates power using cross-sections from the Serpent Monte Carlo code. We report the application of TRACE-PARCS to the primary and secondary circuits of the Molten Salt Fast Reactor, and compare the results with alternative multi-physics tools. Reasonable agreement is found, which paves the way for whole-plant simulations including tertiary turbine circuits.

**Key words:** Multi-physics, molten salt reactor, TRACE, PARCS

## 1. Introduction

Liquid-fuel nuclear reactors have enjoyed significant interest ever since the concept was first conceived some 70 years ago. There are many reasons for this, including tantalising prospects in areas of safety, economics, waste management, and sustainability. In 2002 this interest was reaffirmed with the selection of the molten salt reactor (MSR) as one of six advanced nuclear reactor designs to be further researched and developed by the Generation IV Forum [1]. Currently, these research efforts are focused on the Molten Salt Fast Reactor (MSFR) and are being coordinated and pursued within the Horizon 2020 SAMOFAR (Safety Assessment of the MOlten salt FAst Reactor) project [2].

Despite much interest, considerable challenges remain to be solved for liquid-fuel fast reactors. Among these is the strong interdependency between THs and neutronics that arises from combining the fuel and the coolant into the same liquid. As a result, coupled multi-physics tools are required to simulate dynamic behaviour. Presently, most such tools use computational fluid dynamics (CFD) to solve the TH problem [3, 4, 5, 6]. In this paper, a more lightweight approach is considered in which the system code TRACE is used to solve a simplified set of the TH equations on a coarse computational mesh. Hence, accuracy is compromised for reduced computational requirements.

The presented work builds on previous achievements of the Paul Scherrer Institut [7, 8]. Its novelty is in the explicit coupling between TRACE and the spatial neutron kinetics code PARCS, in combination with the application to liquid-fuel fast reactors with large and open reactor cores that exhibit complex flow patterns. Specifically, we report the application of the coupled TRACE-PARCS tool to the primary and secondary circuits of the MSFR.

## 2. The Molten Salt Fast Reactor

### 2.1. Concept

Figure 1 illustrates the conceptual design of the MSFR, while table I presents the main properties. The reactor uses the thorium fuel cycle, and produces fissile $^{233}$U in the breeding blankets.

| Parameter | Value |
|---|---|
| Power | 3 $GW_{th}$ / 1.5 $GW_e$ |
| Salt volume | 18 $m^3$ |
| Salt fraction in core | 50 % |
| # of circulation loops | 16 |
| Nominal flow rate | 18.5 ton/s $\approx$ 4.5 $m^3$/s |
| Nominal circulation time | 4.0 s |
| Inlet / outlet temperature | 973 K / 1073 K |
| Blanket volume | 7.3 $m^3$ |

*TABLE I. Main properties of the MSFR benchmark specification.*

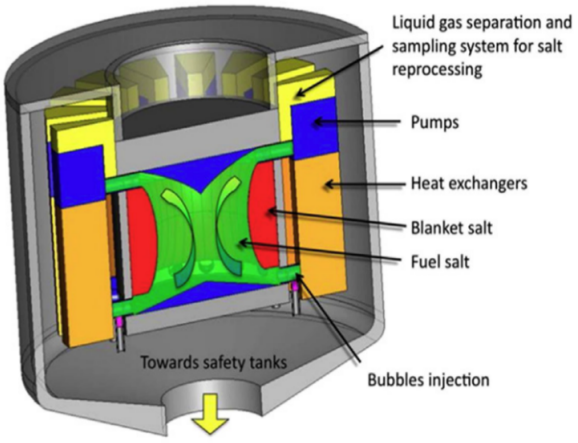



*FIG. 1. Conceptual design of the MSFR [9].*

Both the fuel and blanket salt is the eclectic mixture 77.5LiF-22.5An, where An denotes actinides, primarily $^{232}$Th and $^{233}$U. Table II states the main properties of this salt, which is assumed constant and at beginning-of-life (i.e., no burn-up). The secondary circuit is assumed to use FLiBe.

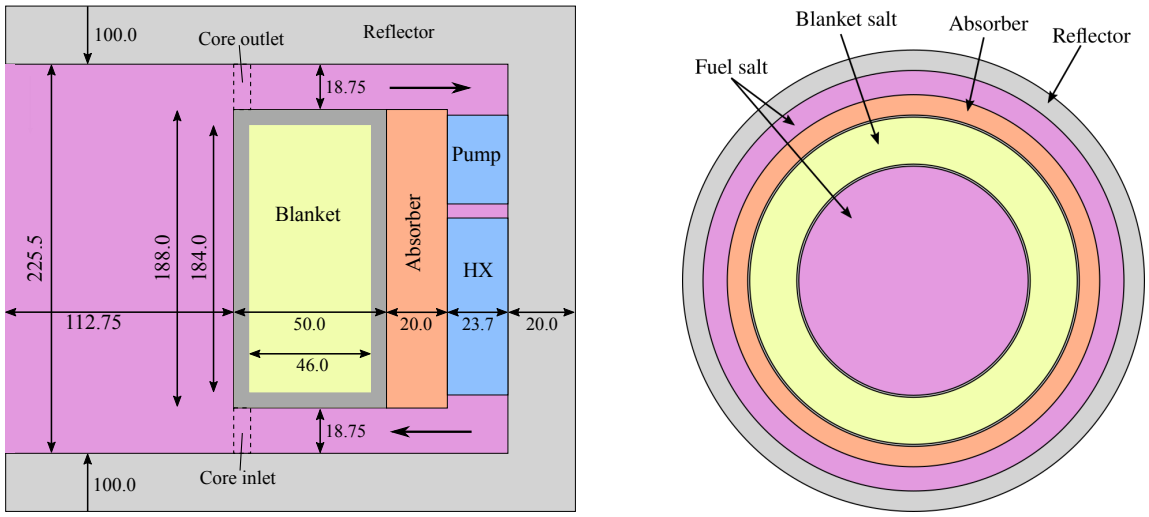
| Property | Symbol | Expression | Validity |
|---|---|---|---|
| Melting temperature [K] | $T_{melt}$ | 841 | 1 bar |
| Boiling temperature [K] | $T_{boil}$ | 1874 | 1 bar |
| Density [kg·m$^{-3}$] | $\rho$ | $4094 - 0.882 \cdot (T - 1024)$ | (893-1125) K |
| Dynamic viscosity [Pa·s] | $\mu$ | $\rho \cdot 5.54 \cdot 10^{-8} \cdot \exp(3689/T)$ | (898-1121) K |
| Thermal conductivity [W·m$^{-1}$·K$^{-1}$] | $k$ | $0.928 + 8.397 \cdot 10^{-5} \cdot T$ | (891-1020) K |
| Specific heat capacity [J·kg$^{-1}$·K$^{-1}$] | $c_p$ | $-1111 + 2.78 \cdot T$ | (867-907) K |

*TABLE II. Experimentally-deduced properties of the LiF-$AnF_4$ (77.5 - 22.5 %-mole) fuel and blanket salt[10]. The properties are assumed to vary negligibly with actinide composition.*

### 2.2. Model Implementation

In this paper, a simplified, axially-symmetric benchmark model of the MSFR has been studied [3, 5, 6, 11]. This consists of the reactor core and one equivalent primary loop representing the 16 individual loops, and including one pump and one heat exchanger. For the determination of macroscopic cross sections in the reactor core, also a blanket salt and $B_4C$ absorber was modelled, but these were neglected in the coupled simulations. Figures 2a and 2b illustrate the benchmark geometry from the side and top, respectively.

For the TH modelling, explicit pump and heat exchanger models were defined. The former was modelled with a built-in centrifugal pump model in TRACE. For the latter, a printed circuit heat exchanger with FLiBe salt on the secondary side was chosen from literature [12].




*(a) Cross-sectional side view.* *(b) Cross-sectional top view.*

*FIG. 2. Illustrations of the axially-symmetric MSFR benchmark geometry. The blanket and absorber regions were neglected in the coupled calculations. All dimensions are in centimetres. Note that (a) is not to scale. Core inlet and outlet are indicated as referred to later on.*

## 3. Tools

Three codes have been used in the preparation of this paper, namely Serpent (v. 2.1.26), TRACE (v. 5.0p3), and PARCS (v. 3.2). The Monte Carlo code Serpent [13] was used to generate macroscopic cross sections for use with the spatial neutron kinetics solver PARCS [14]. PARCS solves the six-group diffusion equation and uses cross section derivatives to account for reactivity variations from temperature changes in relation to a reference temperature. These derivatives were also calculated with Serpent, and are formulated as

$$\left(\frac{\partial \Sigma_x}{\partial T}\right)_T = \frac{\Sigma_{x,T_1} - \Sigma_{x,T_0}}{\ln T_1 - \ln T_0}, \tag{1}$$

for the Doppler feedback derivatives, and

$$\left(\frac{\partial \Sigma_x}{\partial T}\right)_\rho = \frac{\Sigma_{x,T_1} - \Sigma_{x,T_0}}{T_1 - T_0}, \tag{2}$$

for the fuel density feedback derivatives. As a result of these formulations, a temperature range must be selected for calculating the derivatives. In this work, $T_0 = 900$ K and $T_1 = 1200$ K have been used, and $T_0$ has been taken as reference temperature.

TRACE [15] is a THs solver that employs a system code approach to solving the fluid dynamics equations. That means that it solves a simplified set of equations on a comparatively coarse computational mesh. Of particular note is the formulation of the momentum and energy conservation equations, the former given as

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \cdot \boldsymbol{u}) + \nabla p = \boldsymbol{f_w} + \rho \boldsymbol{g}, \tag{3}$$

where the wall friction factor

$$\boldsymbol{f_w} = C_w \boldsymbol{u}|\boldsymbol{u}| = k_w \frac{2\rho}{D_h} \boldsymbol{u}|\boldsymbol{u}|, \tag{4}$$

is an engineering correlation that does not consider turbulence effects nor viscous shear stresses. The energy conservation equation is similarly defined. Moreover, TRACE nominally assumes slip velocity boundary conditions on walls.

In liquid-fuel reactors, delayed neutron precursors (DNPs) are transported with the fuel around the primary circuit. At PSI, a source code extension to TRACE has been undertaken to model this phenomenon [7]. Specifically, it implements a solution routine for the expression

$$\frac{\partial(\rho c_j)}{\partial t} + \nabla \cdot (\boldsymbol{u}\rho c_j) = \nabla \cdot (D_{m,j}\rho \nabla c_j) + \rho(\beta_j n - \lambda_j c_j), \tag{5}$$

where $j$ denote DNP groups.

### 3.1. Coupling Methodology

The coupling between TRACE and PARCS is based on an operator splitting approach. In each time step, the TH problem is solved by TRACE and the temperature and DNP distributions are transferred to PARCS. PARCS then calculates the power deposition which is returned to TRACE and used to re-calculate the THs and DNP distributions in the next time step.

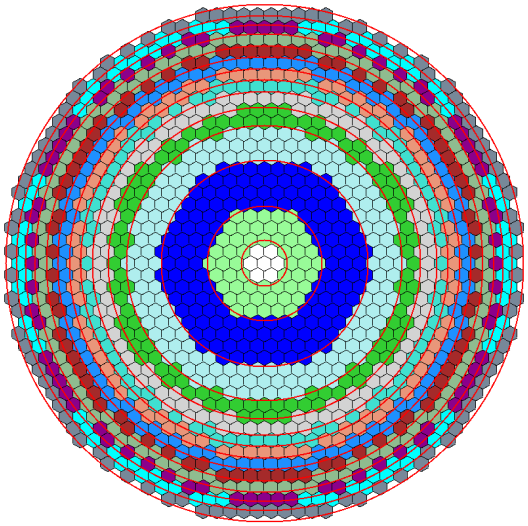


*FIG. 3. The radial discretisation of the MSFR core (inner salt circle in figure 2b) in PARCS overlaid with the TRACE discretisation (red, circular lines) illustrating the coupled regions in which variables are mapped and transferred from one code to the other.*

Since TRACE and PARCS use different computational meshes, a mapping procedure is required to transfer information between the two codes. In PARCS, the radial reactor core mesh consists of 1285 hexagonal cells. These are mapped to the 14 cylindrical cells in TRACE according to the scheme illustrated in figure 3. In the horizontal direction, one-to-one mapping has been used.

## 4. Results

Steady-state and transient simulations of the MSFR have been performed. The former progressed in an uncoupled manner, and was required in order to initialise the transient simulations with the coupled tool.

### 4.1. Steady-State

Steady-state calculations were performed with both PARCS and TRACE, and comparisons were made with other code systems. For the neutronic calculations, Serpent has been used as reference, while the THs comparison have been made with results from the CFD tool COMSOL [16] available in the literature [3].

Table III lists the $k_{\text{eff}}$ at a uniform core temperature of $T = 1030$ K[1] together with the reactivity temperature coefficients calculated by Serpent and PARCS. In general, the agreement is quite good. The difference in $k_{\text{eff}}$ is about 100 pcm, and around 1-2 % for the temperature coefficients. For obtaining the PARCS results, it has been assumed that the total temperature coefficient can be approximated as the sum of the Doppler and salt density coefficients. Table III also shows that this approximation is justified.

| Code | $k_{\text{eff}}$ | $\alpha_D$ [pcm/K] | $\alpha_\rho$ [pcm/K] | $\alpha_D + \alpha_\rho$ [pcm/K] | $\alpha_T$ [pcm/K] |
|---|---|---|---|---|---|
| Serpent | 1.00000 | -3.88 $\pm$ 0.02 | -3.48 $\pm$ 0.02 | -7.36 $\pm$ 0.03 | -7.27 $\pm$ 0.02 |
| PARCS | 0.99917 | -3.87 | -3.59 | -7.46 | -7.63 |

*TABLE III. Neutron multiplication factor at* T = 1030 *K and reactivity coefficients as calculated by PARCS and Serpent. See the nomenclature for explanation of symbols. The coefficients have been calculated as* $\alpha = (k_{eff,1} - k_{eff,0})/(k_{eff,0} \cdot \Delta T)$*, with* $k_{eff,0} = k_{eff,\ 900\ K}$*,* $k_{eff,1} = k_{eff,\ 1200\ K}$*, and* $\Delta T = 300$ *K.*

Some calibration of PARCS was performed by adjusting the albedo boundary condition to obtain the same $k_{\text{eff}}$ as Serpent at a uniform core temperature of $T_0 = 900$ K.

Calibration was also required to compare TRACE with COMSOL. The core inlet and outlet temperatures were aligned with COMSOL by modifying the mass flow rates on the secondary and primary sides, respectively. Since TRACE and COMSOL were found to use different fuel salt heat capacities (1594 vs. 1355 J/kg/K), TRACE predicted a 30% higher mass flow[2]. The core peak temperature could be tuned by modifying friction parameters to resemble the viscous shear stresses and turbulent effects in COMSOL. The resulting velocity and temperature distributions are illustrated in figures 4 and 5.

Although significant discrepancies are present, TRACE is able to reproduce the general trends of the COMSOL results. This includes the large and nearly stagnant recirculation zone close to the breeding blanket. Conversely, the size of the recirculation zone is greater in COMSOL so that circulating salt has to flow faster in the remaining flow area. In addition, the core average temperature in COMSOL ($\sim$1070 K) is appreciably higher than in TRACE ($\sim$1030 K).

In summary, it is clear that TRACE is not able to reproduce the same level of detail as COMSOL. However, considering the fundamental simplifications and coarser mesh used in TRACE, the agreement is reassuringly good and found to be sufficient for the purpose of this study.

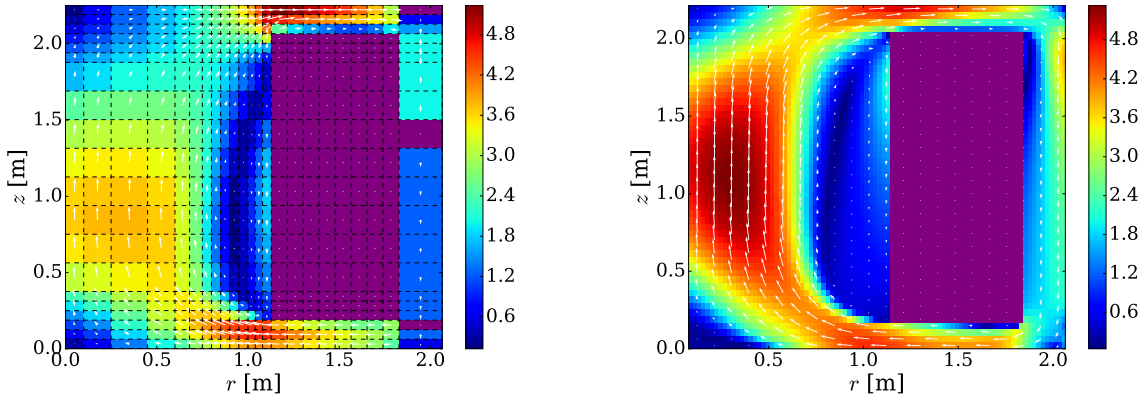
### 4.2. Transients

Simulations of two accidental transients postulated for the MSFR are presented in the below; the unprotected loss of heat sink (ULOHS) and unprotected over-cooling (UOC). To assess the ability of the coupled tool to accurately predict the dynamic behaviour of the MSFR, the results have been compared with two other tools. These are a TRACE-based solver that has

[1] 1030 K represents a volume-averaged core temperature determined from preliminary TRACE simulations.

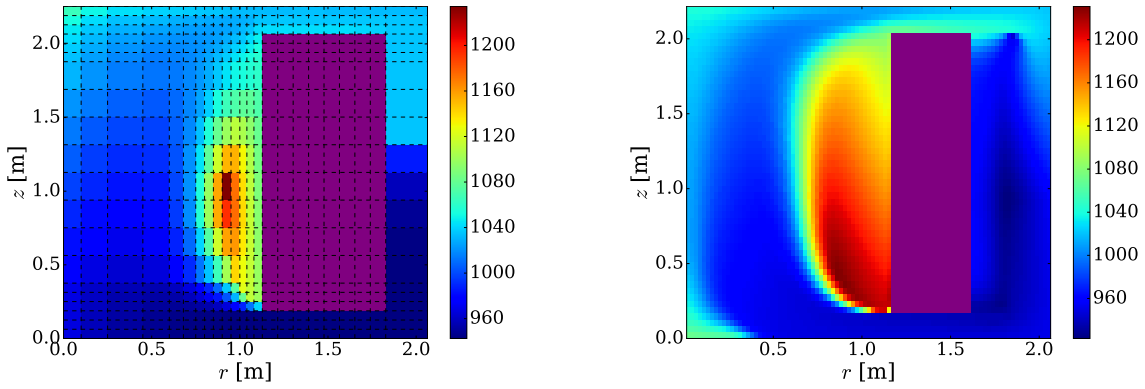
[2] This difference in $c_p$ was also present between TRACE-PARCS and the other coupled tools considered herein.

been extended with a point kinetics solver routine [7] (hereby referred to as 'TRACE-PK') and a COMSOL tool that makes use of a spatial diffusion solver [3] (referred to as 'COMSOL').




*(a)* *(b)*

*FIG. 4. MSFR velocity field [m/s] as calculated by **(a)** TRACE and **(b)** COMSOL. Since 3 $GW_{th}$ are produced in the core and removed in the heat exchanger in both models, and because the heat capacity is lower in TRACE, the total mass flow is about 30% higher in TRACE.*




*(a)* *(b)*

*FIG. 5. MSFR temperature field [K] as calculated by **(a)** TRACE and **(b)** COMSOL. The higher average temperature in COMSOL is mostly from the larger stagnant zone that comes from modelling turbulence.*

### 4.2.1 Unprotected Loss of Heat Sink

The ULOHS scenario has been simulated with TRACE, TRACE-PK, and COMSOL by disabling the heat transfer in the heat exchanger at $t = 0$. The resulting temperature, power, and core inlet-outlet temperature difference (denoted $\Delta T$) are illustrated in figures 6 and 7.

The three tools agree on the general dynamics of the transient. As the primary circuit salt heats up, the negative temperature feedback ensures that the power level is decreased towards zero. Since the reactor is taken to be adiabatic, the temperature uniformly increases towards an asymptotic value. At the same time, $\Delta T$ approaches zero as the temperature distribution becomes uniform. This approach to zero is characterised by damped oscillations that result from locally heated or cooled blobs of circulating salt.

The most striking discrepancy between the three tools is the average core temperature. This is initially greater in COMSOL because of the larger recirculation zone. As the transient unfolds, it also increases the most in the COMSOL simulation. The smallest temperature increase is

predicted by TRACE-PARCS because the removal of heat exchange occurs instantaneously at $t = 0$, whereas for TRACE-PK and COMSOL it is removed following an exponential decay with a time constant of 1.0 s. Consequently, less thermal energy is released in the salt before the chain reaction stops (equal to the integral under the power graph) in the TRACE-PARCS simulation.

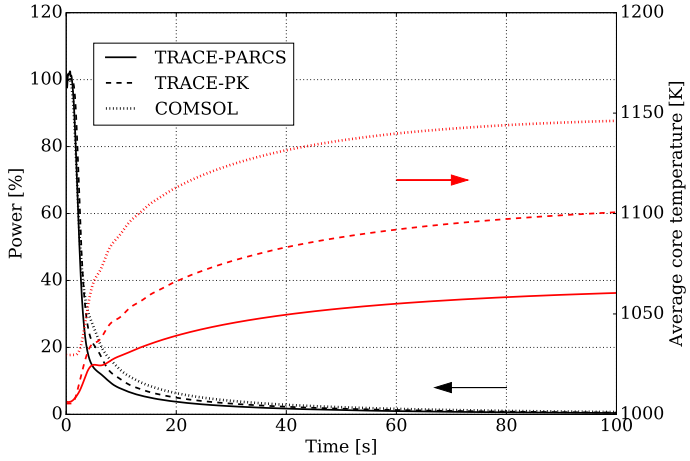



*FIG. 6. Power (black) and average core temperature (red) versus time as calculated by TRACE-PARCS, TRACE-PK, and COMSOL for the ULOHS transient.*

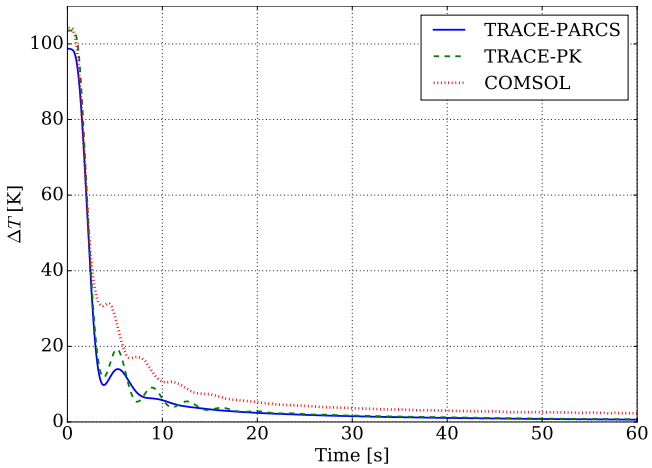



*FIG. 7.* $\Delta T = T_{core,outlet} - T_{core,inlet}$ *as a function of time as calculated by TRACE-PARCS. TRACE-PK, and COMSOL for the ULOHS transient.*

### 4.2.2 Unprotected Over-Cooling

To produce electricity, an MSFR plant must feature a pressurised tertiary circuit which could cause excessive cooling of the primary circuit if inadvertently and rapidly depressurised. Such UOC transient has been simulated herein by reducing the inlet temperature on the secondary side of the heat exchanger by 70 K. As a result, the core inlet temperature (c.f. figure 2a) was reduced by about 45 K.

The three tools generally agree on the transient behaviour. As cool salt first enters the core, the reactivity insertion causes the power to increase. Eventually, a new equilibrium between heat generation and removal is established at an elevated power level.

As before, there are significant discrepancies in the evolution of the average core temperature. Both TRACE-PK and TRACE-PARCS compute an overall increase, while COMSOL predicts

a decrease. This indicates that the recirculation zone has been disturbed in COMSOL. A similar disturbance could also be causing the initial decrease in the TRACE-PK simulation. In both cases, full data sets of core temperature distributions versus time are needed to establish the exact cause. In contrast, TRACE-PARCS displays only a very small decrease initially and a stable recirculation zone throughout.

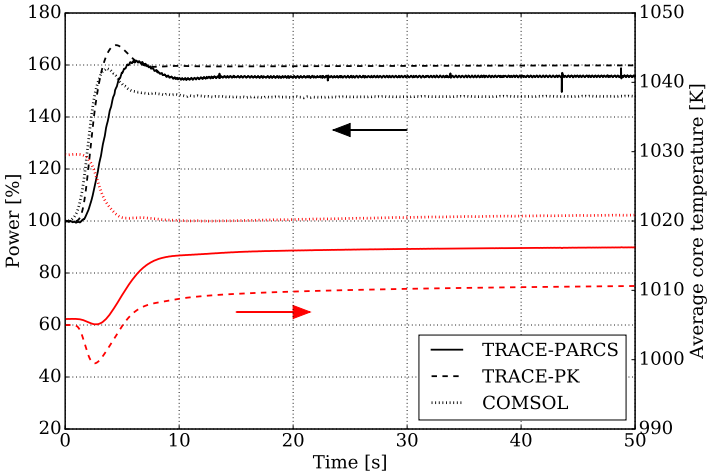



*FIG. 8. Power (black) and average core temperature (red) versus time as calculated by TRACE-PARCS, TRACE-PK, and COMSOL for the UOC transient. The transient begins a bit later in TRACE-PARCS because of differences in the heat exchanger models implemented.*

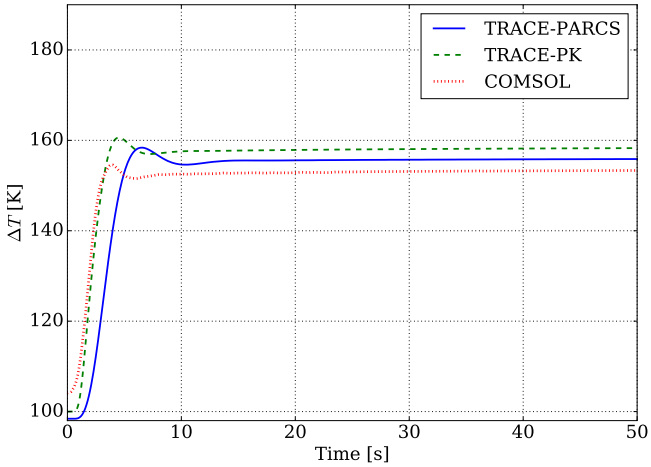



*FIG. 9.* $\Delta T = T_{core,outlet} - T_{core,inlet}$ *as a function of time as calculated by TRACE-PARCS, TRACE-PK, and COMSOL for the UOC transient.*

## 5. Conclusions and Outlook

This paper has presented a new, coupled multi-physics solver for simulating circulating-fuel fast reactors. The tool consists of the THs system code TRACE together with the spatial neutron kinetics solver PARCS, and uses macroscopic cross sections generated by the Monte Carlo code Serpent. Its main features include a coarse mesh and simplified equations solution strategy that lowers computational requirements compared to CFD solvers, and a dedicated DNP drift model.

The coupled TRACE-PARCS tool has been applied to transient analysis of the MSFR. In general, it produces results that are in reasonable agreement with two alternative multi-physics solvers, including one of higher complexity. Significant discrepancies do exist, particularly in the calculation of the average core temperature, however, this is also true between the two

alternative tools. As such, this highlights the computational challenge of simulating highly interdependent, multi-physics systems that ideally require both high resolution and accurate boundary conditions.

In terms of computational requirements, TRACE-PARCS does not greatly improve on the performance of CFD-based solvers. Although it could be executed on a single CPU, run times were prohibitively long and frequently stretched to several days. Some acceleration techniques are suggested for improving this. First, parallel computing can be enabled through domain decomposition. Second, the computational mesh used in PARCS can likely be reduced with little loss in computational accuracy. Third, the source code extensions to TRACE should be further optimised. Fourth, symmetry considerations of the problem geometry can be utilised in PARCS so long as asymmetrical transients are not investigated.

Ultimately, TRACE-PARCS has been found to represent a viable tool for simulating circulating-fuel fast reactors when computational resources are scarce or the considered model is large. The presented work thus paves the way for further investigation of circulating-fuel fast reactors, and, with acceleration techniques, allows for straightforward extensions to full plant modelling and asymmetric transient investigation.

## Acknowledgements

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**Nomenclature**

| | | | |
|---|---|---|---|
| $c_j$ | concentration of DNP group $j$ | $\alpha_D$ | Doppler reactivity coefficient |
| $C_w$ | wall drag coefficient | $\alpha_T$ | overall temperature reactivity coefficient |
| $D_{m,j}$ | molecular diffusivity of DNP group $j$ | $\alpha_\rho$ | fuel salt density reactivity coefficient |
| $f_w$ | wall friction force (per volume) | $\beta_j$ | delayed neutron fraction for DNP group $j$ |
| $g$ | gravitational constant | $\Delta T$ | Core inlet and outlet temperature difference |
| $k_{\text{eff}}$ | neutron multiplication factor | $\lambda_j$ | decay constant for DNP group $j$ |
| $k_w$ | Churchill correlation friction factor | $\rho$ | density |
| $n$ | neutron density | $\Sigma$ | macroscopic cross section |
| $p$ | pressure | | |
| $t$ | time | | |
| $T$ | temperature | | |
| $u$ | fluid velocity | | |

Boldface indicates vector quantities.