



Multiphysics analysis of RANS-based turbulent transport of solid fission products in the Molten Salt Fast Reactor

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ABSTRACT

The analysis of innovative reactor concepts such as the Molten Salt Fast Reactor (MSFR) requires the development of new modeling and simulation tools. In the case of the MSFR, the strong intrinsic coupling between thermal–hydraulics, neutronics and fuel chemistry has led to the adoption of the multiphysics approach as a state-of-the-art paradigm. One of the peculiar aspects of liquid-fuel reactors such as the MSFR is the mobility of fission products (FPs) in the reactor circuit. Some FP species appear in form of solid precipitates carried by the fuel flow and can deposit on reactor boundaries (e.g., heat exchangers), potentially representing design issues related to the degradation of heat exchange performance or radioactive hotspots. Other precipitates might be present in the primary system as well, e.g. due to oxidation of fissile species which might lead to local criticality issues. The integration of transport models for solid particles in multiphysics codes is therefore relevant for the prediction of deposited fractions. To this aim, a previously developed Eulerian single-phase transport model is employed to analyze the distribution of solid FPs in two simplified MSFR-related geometries. The effect of physical parameters and of distributed particle sources on the numerical requirements needed to resolve particle concentration gradients at reactor boundaries in the considered geometries is investigated with the aid of analytical results. Analytical estimates of concentration gradients, even though not in full agreement with simulations, prove useful to drive the choice of adequate mesh refinements. Furthermore, the influence of different RANS turbulence modeling approaches on the prediction of particle distributions and deposition is tested. Results show a limited influence of the choice of turbulence models and parameters on the deposited fraction and on concentration gradients. As a result, it is found that deposition rates are scarcely affected by the choice of turbulent Schmidt number, with lower diffusivities being compensated by larger gradients. Large deposited fractions are indeed predicted, suggesting the efficiency of FPs transport mechanisms in the reactor and the need for the integration of adequate FPs transport models within state-of-the-art MSFR codes.

1. Introduction

The interest towards liquid-fuel reactor concepts has seen a significant increase over the last years. Among them, the fast-spectrum MSFR (Molten Salt Fast Reactor) (Serp et al., 2014), which was featured among the selected Generation IV reference technologies, has gained a leading role in the molten salt reactor research field thanks to its innovative design. The tight coupling among thermal–hydraulics, neutronics and fuel chemistry due to fuel circulation makes the MSFR system unique from the design and modeling viewpoints. The multiphysics approach has therefore become the standard tool for the development of computational models and to address the design and analysis of the MSFR (Tiberga et al., 2020). Multiphysics simulation codes have been

successfully employed to address several MSFR features, such as for instance the adoption of a bubbling system (Cervi et al., 2019), fuel compressibility effects (Cervi et al., 2019), the analysis of freeze-valve behavior (Tiberga et al., 2019). Multiphysics-based MSFR models have also been adopted to test the application of advanced data analysis and model order reduction techniques (German et al., 2020; Di Ronco et al., 2020).

Fission products (FPs) represent a major challenge in the modeling and design of the MSFR. They originate within the fuel and are not retained by solid structures, being thus free to be carried by the liquid fuel along the primary circuit. Some FP species are not expected to form stable compounds with the constituents of the fuel salt mixture (Grimes, 1970; Baes, 1974) and therefore may give rise to separate phases, either in the form of solid precipitates or gas bubbles. Solid FPs are likely to

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Nomenclature**Latin symbols**

$A_{r,g}^0$	reference g -th group, r -th neutron reaction cross-section
	log. coeff.
C	particle (vol.) concentration
C_d	deposited particle (surf.) concentration
c_k	k -th family del. neutron prec. (vol.) concentration
c_p	fluid specific heat capacity
d_l	l -th family decay heat prec. (vol.) concentration
d_p	particle diameter
D	laminar particle diffusivity
D_{eff}	effective particle diffusivity
$D_{n,g}$	g -th group neutron diffusion coefficient
D_t	turbulent particle diffusivity
Da	Damköhler number
$\bar{E}_{f,g}$	avg. g -th group fission energy
g	gravitational acceleration
H	channel half-width
J_d	particle (surf.) deposition flux
k_B	Boltzmann constant
k_{eff}	effective multiplication factor
p	fluid pressure
Pr	Prandtl number
Pr_t	turbulent Prandtl number
q'''	vol. energy source
S	channel particle (vol.) source
S_{max}	channel max. particle (vol.) source
S_{min}	channel min. particle (vol.) source
Sc	Schmidt number
Sc_t	turbulent Schmidt number
Sh	Sherwood number
T	fluid temperature
T_{sink}	heat sink temperature
T_0	reference temperature (buoyancy)
T_0^Σ	reference temperature (group constants)

\mathbf{u}	fluid velocity
V_r	heat removal region volume
v_g	avg. g -th group neutron velocity
y	channel transversal coord.
γ_C	fission yield of particles

Greek symbols

α	laminar thermal diffusivity
α_{eff}	effective thermal diffusivity
α_t	turbulent thermal diffusivity
β_d	total del. neutrons prec. fraction ($\sum_k \beta_{d,k}$)
$\beta_{d,k}$	k -th family del. neutron prec. fraction
β_h	total decay heat prec. fraction ($\sum_l \beta_{h,l}$)
$\beta_{h,l}$	l -th family decay heat prec. fraction
β_T	vol. thermal expansion coeff.
γ	deposition velocity
γ_r	heat removal coefficient
Δy^*	characteristic wall length
λ_C	particle decay constant
$\lambda_{d,k}$	k -th family del. neutron prec. decay constant
$\lambda_{h,l}$	l -th family decay heat prec. decay constant
ν	laminar kinematic viscosity
ν_{eff}	effective kinematic viscosity
ν_t	turbulent kinematic viscosity
$\bar{\nu}_g$	avg. g -th group neutrons emitted per fission
ρ	fluid density
$\Sigma_{a,g}$	g -th group absorption cross-section
$\Sigma_{f,g}$	g -th group fission cross-section
$\Sigma_{r,g}$	g -th group, r -th neutron reaction cross-section
$\Sigma_{r,g}^0$	reference g -th group, r -th neutron reaction cross-section
$\Sigma_{s,g \rightarrow h}$	g -to- h -th group scattering cross-section
$\chi_{d,g}$	g -th energy group delayed neutron spectrum
$\chi_{p,g}$	g -th energy group prompt neutron spectrum
ϕ_g	g -th group integrated neutron flux

deposit on reactor surfaces in the form of solid precipitates (Kedl, 1972; Compere et al., 1975), giving rise to potential issues such as formation of localized decay heat sources as well as deterioration of heat exchanger performance. Surface deposits might also pose a serious radiological threat in inspection/maintenance operations. In a similar way, the oxidation of fissile species in particular operating conditions might lead to the formation of solid precipitates (Beneš and Konings, 2012), with potential issues related to the transport and local accumulation of fissile particles. The analysis of FPs transport has found limited space in recent MSFR studies. In this regard, there has been focus on modeling the behavior and effects of Xenon transport in MSRs (Price et al., 2020; Caruggi et al., 2022), while the analysis of metallic FPs in the context of a multiphysics system code for the study of the Molten Salt Reactor Experiment has been recently addressed by Walker and Ji (2021). The analysis of the MSFR by means of a traditional system-code approach is made difficult by its peculiar geometry and fuel circulation, making the use of high-fidelity models a more appropriate choice. A first approach for the integration of metallic FPs transport in a CFD-based multiphysics model has been described and verified against simplified analytical solutions in Di Ronco et al. (2021). Such approach is intended to allow for the analysis of inherently two-/three-dimensional effects, such as transport in complex turbulent flows, the estimation of particle deposition fluxes directly from concentration fields and the interaction with the gas bubbling system. Local temperature effects on precipitation of metallic species can also be directly taken into account, in view of

coupling with thermochemistry calculations (Marino et al., 2020).

The aim of this work is therefore the application of transport models for solid FPs integrated in state-of-the-art MSFR multiphysics tools to the preliminary analysis of FPs transport and deposition in relevant two-dimensional MSFR cases. Potential numerical issues arising from the commonly adopted ‘‘perfect adsorption’’ wall boundary conditions are addressed. Analytical results from Di Ronco et al. (2021) are used to illustrate such issues, and are compared to numerical simulation in a lid-driven cavity. Such case has been previously developed and studied in the context of benchmarking activities for multiphysics MSR codes (Tiberga et al., 2020). Then, due to their direct effect on species transport, different turbulence modeling approaches are tested in a more realistic MSFR case. The paper is organized as follows. The adopted multiphysics approach is briefly described in Section 2. The wall deposition problem is discussed, together with its analytical formulation, in Section 3. Section 4 describes the selected application cases, while Section 5 presents the results of the analysis together with some discussion. Conclusive remarks are finally reported in Section 6.

2. Multiphysics model

The OpenFOAM library (OpenFOAM, 2021), based on standard finite-volume methods for CFD calculations, is used to develop the numerical solver used in the present work. Originally developed for the transient analysis of the MSFR (Aufiero et al., 2014), the adopted

multiphysics solver was recently extended to allow for the study of compressibility effects during super-prompt-critical transients (Cervi et al., 2019) and of the bubbling system (Cervi et al., 2019; Caruggi et al., 2022). The version employed in this work features single-phase incompressible thermal-hydraulics, multi-group neutron diffusion and transport equations for delayed neutron and decay heat precursors. Transport equations for fission products are solved alongside the other physical modules, to provide a fully-coupled multiphysics simulation. All model equations are solved by means of finite-volume discretization, following an iterative segregated coupling approach.

2.1. Thermal-hydraulics model

Continuity, momentum and energy (in temperature form) conservation equations are expressed in a single-phase incompressible formulation:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}^T) = -\frac{1}{\rho} \nabla p + [1 - \beta_T(T - T_0)] \mathbf{g} + \nabla \cdot [\nu_{eff} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] \quad (2)$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u} T) = \nabla \cdot (\alpha_{eff} \nabla T) + \frac{q'''}{\rho c_p} \quad (3)$$

where the quantities \mathbf{u}, p and T , which correspond to velocity, pressure and temperature, respectively, are intended as averaged in the sense of Reynolds-Averaged Navier–Stokes modeling. It follows that turbulence modeling is performed by means of standard linear eddy-viscosity based closure models, for which effective momentum and thermal diffusivities can be expressed as the sum of a laminar and a turbulent contribution:

$$\nu_{eff} = \nu + \nu_t \quad (4)$$

$$\alpha_{eff} = \alpha + \alpha_t = \frac{\nu}{Pr} + \frac{\nu_t}{Pr_t} \quad (5)$$

where Pr and Pr_t are the Prandtl and turbulent Prandtl numbers, respectively. Momentum and energy equations are coupled thanks to the Boussinesq approximation, for which the density value driving the buoyancy term in Eq. (2) is linearized around a reference temperature T_0 and β_T represents the volumetric thermal expansion coefficient of the fluid. Except for what concerns density in the linearized buoyancy term, constant average values are used for thermophysical properties to keep the numerics and the coupling between different physics as simple as possible. Finally, q''' represents a volumetric energy source which includes internal heat generation (both prompt and delayed, see Eq. (10)) and optionally other energy sinks to model heat removal mechanisms.

2.2. Neutronics model

The multi-group diffusion model is adopted for neutron flux calculations (Hébert, 2010). Despite some limitations, it is widely employed in standard nuclear reactor analysis. Thanks to its relative simplicity and limited computational effort, it has found several successful applications especially for multiphysics analysis (Aufiero et al., 2014; Fiorina et al., 2016). More recent works have also proposed the extension of OpenFOAM-based multiphysics codes to more advanced neutron transport approaches, e.g. the SP3 model (Fiorina et al., 2017; Cervi et al., 2019). The diffusion equation for the g -th group-integrated neutron flux φ_g reads:

$$\frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} = \nabla \cdot (D_{n,g} \nabla \varphi_g) - \Sigma_{a,g} \varphi_g - \sum_{h \neq g} \Sigma_{s,g \rightarrow h} \varphi_h + (1 - \beta_d) \chi_{p,g} \frac{\bar{v}_g}{k_{eff}} \Sigma_{f,g} \varphi_g + S_{n,g} \quad (6)$$

where $S_{n,g}$ is the explicit neutron source of the g -th group, constituted by prompt fission and scattering neutrons from other groups and delayed neutron precursors decay:

$$S_{n,g} = (1 - \beta_d) \sum_{h \neq g} \chi_{p,h} \frac{\bar{v}_h}{k_{eff}} \Sigma_{f,h} \varphi_h + \sum_{h \neq g} \Sigma_{s,h \rightarrow g} \varphi_h + \chi_{d,h} \sum_k \lambda_{d,k} c_k \quad (7)$$

The presence of φ_h in the explicit source term $S_{n,g}$ couples the transport equations for different energy groups, which are therefore dealt with following a segregated iterative approach. Most symbols have straightforward meaning and are listed in the Nomenclature section. It is worth mentioning that k_{eff} acts as a tunable multiplication factor to model a prescribed reactivity insertion. A power-iteration routine for the solution of the k -eigenvalue problem is also included for steady-state simulation, which allows for the iterative adjustment of k_{eff} to attain criticality at a specified power level.

Due to the circulating nature of the fuel, transport equations are formulated also for delayed neutron and decay heat precursors. The transport equation for the concentration of delayed neutron precursors of the k -th family c_k reads:

$$\frac{\partial c_k}{\partial t} + \nabla \cdot (\mathbf{u} c_k) = \nabla \cdot (D_{eff} \nabla c_k) - \lambda_{d,k} c_k + \beta_{d,k} \sum_g \bar{v}_g \Sigma_{f,g} \varphi_g \quad (8)$$

An analogous equation holds for the concentration of decay heat precursors of the l -th family d_l :

$$\frac{\partial d_l}{\partial t} + \nabla \cdot (\mathbf{u} d_l) = \nabla \cdot (D_{eff} \nabla d_l) - \lambda_{h,l} d_l + \beta_{h,l} \sum_g \bar{E}_{f,g} \Sigma_{f,g} \varphi_g \quad (9)$$

In the above equation, the actual concentration of decay heat precursors is multiplied by the average fission energy, such that d_l represents a volumetric amount of “latent” fission energy. Consistently, the volumetric heat source is given by:

$$q''' = (1 - \beta_h) \sum_g \bar{E}_{f,g} \Sigma_{f,g} \varphi_g + \sum_l \lambda_{h,l} d_l \quad (10)$$

For what concerns the diffusive transport of delayed neutrons and decay heat precursors, the diffusion coefficient D_{eff} is simply defined in analogy with momentum and thermal diffusivities as in Eq. (4 and 5):

$$D_{eff} = D + D_t = \frac{\nu}{Sc} + \frac{\nu_t}{Sc_t} \quad (11)$$

where Sc and Sc_t are the Schmidt and turbulent Schmidt numbers, respectively.

Group constants are adjusted as functions of local temperature around reference values to account for Doppler and fuel density effects. For a generic neutron reaction r occurring in the g -th energy group:

$$\Sigma_{r,g} = \left(\Sigma_{r,g}^0 + A_{r,g}^0 \log \frac{T}{T_0^0} \right) \frac{1 - \beta_T(T - T_0)}{1 - \beta_T(T_0^0 - T_0)} \quad (12)$$

where Doppler effects are modeled by means of a logarithmic term where $\Sigma_{r,g}^0$ and $A_{r,g}^0$ respectively represent the cross-section and a corresponding logarithmic coefficient at a reference temperature T_0^0 , whereas density effects are taken into account through a linear correction consistently with the buoyancy term. The reference temperature for cross-sections can be chosen independently from T_0 . An analogous approach is employed for the correction of the intra-group neutron diffusion coefficient $D_{n,g}$. The quantities $\Sigma_{r,g}^0$ and $A_{r,g}^0$ are evaluated by means of the Monte Carlo reactor physics and burnup code SERPENT 2 (Leppänen et al., 2015).

2.3. Fission products transport model

Each fission product specie is modeled as a continuous scalar concentration field subject to advection, dispersion and decay mechanisms:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) = \nabla \cdot (D_{\text{eff}} \nabla C) - \lambda_C C + y_C \sum_g \Sigma_{f,g} \phi_g \quad (13)$$

where C is the concentration of the species under consideration, expressed in number of particles per unit volume. Since we neglect chemical interactions and formation of separate phases, the source term is simply related to the fission rate through a suitable yield coefficient y_C .

The single-phase Eulerian approach is employed to limit the additional complexity of the computational model. It represents a valid approximation in many cases of interest, provided that particles are sufficiently small and do not interact among themselves (Guha, 2008). Previous experience with MSRs (Compere et al., 1975) suggests the validity of such modeling choice, at least at a first degree of approximation. The particle size can be used to derive a common expression for the laminar diffusivity D , which is given by the so-called Stokes–Einstein equation:

$$D = \frac{k_B T}{3\pi\rho\nu d_p} \quad (14)$$

where k_B is the Boltzmann constant and d_p is the particle diameter. The above equation is derived under the assumption of large Schmidt number Sc (Balboa Usabiaga et al., 2013) and can be used to estimate Sc in such limit:

$$Sc = \frac{3\pi\rho\nu^2 d_p}{k_B T} \quad (15)$$

It is worth mentioning that particle size plays a relevant role in determining particle diffusivity, according to the Stokes–Einstein relation. Particles sizes are determined by complex nucleation and growth mechanisms. Furthermore, size influences the relative role of inertial effects on momentum transport, invalidating the assumption of gradient-driven turbulent transport above certain diameter values. For the sake of simplicity, these modeling aspects are here neglected. In this work, we focus on the role of turbulence modeling on particle transport and we defer a sensitivity analysis on Sc to future developments.

As shown in (Di Ronco et al., 2021), particle–wall interaction mechanisms can be modeled separately from the bulk flow. This approach, which is valid under fairly general hypotheses on the nature of particle–wall interactions, assumes that relevant interactions only occur in a thin wall region whose influence can be collapsed in a first-order boundary conditions for the bulk flow (Prieve and Ruckenstein, 1976):

$$-D_{\text{eff}} \nabla C \cdot \mathbf{n} = \gamma C \quad (16)$$

for any point on the wall boundary, where \mathbf{n} denotes the outward pointing wall-normal direction. In this model, wall adsorption of FP particles is modeled through a single deposition parameter γ , which has the physical dimensions of a velocity.

3. Particle deposition with distributed sources

Before proceeding to the analysis of application cases, we discuss here some peculiar aspects of problems involving the transport of quantities subject to deposition boundary conditions and distributed internal generation. Distributed internal generation represents a modelling condition which is hardly found in common particle transport problems, and its effects on the concentration boundary layer need to be carefully addressed in CFD-based calculations. In particular, it is found that when deposition boundary conditions prescribe a vanishing species concentration at wall boundaries, large concentration gradients are to be expected if non-negligible generation of particles occurs in the boundary layer. This is naturally the case in MSFR calculations, where the fission rate does not vanish at reactor boundaries.

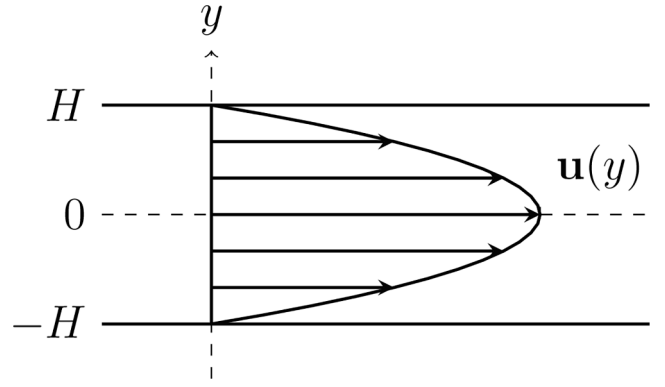


Fig. 1. Parallel plates channel geometry: with respect to the flow, the y coordinate denotes the transversal direction. Wall boundaries are located at $y = \pm H$.

To provide insight on this issue, analytical solutions for the scalar transport problem defined by Eq. (13) are found for simplified test cases. Albeit simplified, these results are useful to understand general features of expected solutions of more complex problems. The fully-developed parallel-plates transport problem Eq. (13) reduces to the 1D equation

$$D_{\text{eff}} \frac{d^2 C}{dy^2} - \lambda_C C + S(y) = 0 \quad (17)$$

equipped with the boundary conditions

$$\mp D_{\text{eff}} \frac{dC}{dy} = \gamma C, \quad y = \pm H \quad (18)$$

Here, y denotes the coordinate in the direction transversal to the channel-flow, and H is the half-width of the channel (Fig. 1).

The solution for a cosine-shaped source of the form

$$S(y) = S_{\min} + (S_{\max} - S_{\min}) \cos\left(\frac{\pi}{2H} y\right) \quad (19)$$

reads

$$C(y) = \left(\frac{S_{\max}}{\lambda_C}\right) K \left(e^{\frac{\sqrt{Da}}{H} y} + e^{-\frac{\sqrt{Da}}{H} y} \right) + \left(\frac{S_{\max}}{\lambda_C}\right) \left[\left(\frac{S_{\min}}{S_{\max}}\right) + \left(1 - \frac{S_{\min}}{S_{\max}}\right) \frac{4Da}{4Da + \pi^2} \cos\left(\frac{\pi}{2H} y\right) \right] \quad (20)$$

where

$$K = \frac{-\left(\frac{S_{\min}}{S_{\max}}\right) Sh + \left(1 - \frac{S_{\min}}{S_{\max}}\right) \left(\frac{\pi}{2}\right) \frac{4Da}{4Da + \pi^2}}{Sh(e^{\sqrt{Da}} + e^{-\sqrt{Da}}) + \sqrt{Da}(e^{\sqrt{Da}} - e^{-\sqrt{Da}})} \quad (21)$$

Non-dimensional quantities have been defined as $Sh = \gamma H / D_{\text{eff}}$ and $Da = \lambda_C H^2 / D_{\text{eff}}$. Introducing some additional hypotheses, such as $Sh \gg \sqrt{Da} \gg 1$, it is possible to further simplify the solution:

$$C(y) = \left(\frac{S_{\max}}{\lambda_C}\right) \left\{ \left(\frac{S_{\min}}{S_{\max}}\right) \left[1 - \frac{e^{\frac{\sqrt{Da}}{H} y} + e^{-\frac{\sqrt{Da}}{H} y}}{e^{\sqrt{Da}} + e^{-\sqrt{Da}}} \right] + \left(1 - \frac{S_{\min}}{S_{\max}}\right) \cos\left(\frac{\pi}{2H} y\right) \right\} \quad (22)$$

The role of the ratio S_{\min}/S_{\max} appears evident when considering the two extreme cases:

(A) $S_{\min}/S_{\max} \rightarrow 0$: the concentration profile tends to a simple cosine shape:

$$C(y) \rightarrow \left(\frac{S_{\max}}{\lambda_C}\right) \cos\left(\frac{\pi}{2H} y\right) \quad (23)$$

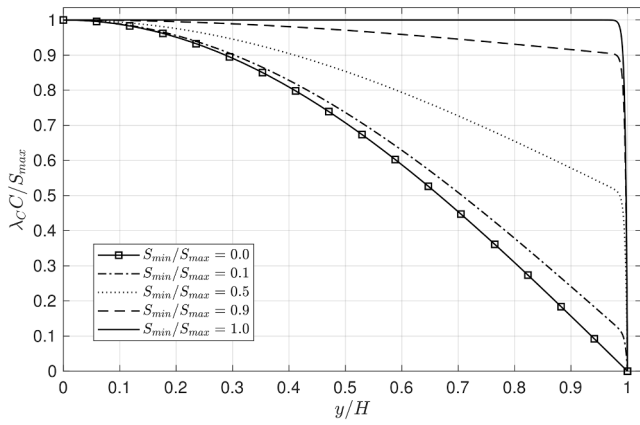


Fig. 2. Analytical solutions for the 1D parallel plates geometry. Different S_{min}/S_{max} ratios produce similar behaviors: the concentration profiles follow a cosine-shaped profile in the bulk flow, then drop to 0 in a thin region close to the wall boundary. The thickness Δy^* shows little dependence on S_{min}/S_{max} . For these cases, $Da = 80000$.

(B) $S_{min}/S_{max} \rightarrow 1$: the concentration profile tends to a uniform shape, except for a thin wall region where it quickly drops to 0:

$$C(y) \rightarrow \left(\frac{S_{max}}{\lambda_C} \right) \left(1 - \frac{e^{-\frac{\sqrt{Da}}{H}y} + e^{-\frac{\sqrt{Da}}{H}(H-y)}}}{e^{\sqrt{Da}} + e^{-\sqrt{Da}}} \right) \quad (24)$$

Cases sufficiently far from (A) are significant for realistic reactor applications, where the “perfectly absorbing walls” condition ($Sh \gg 1$) is assumed to adequately approximate particle–wall interactions and the distributed source does not vanish close to walls. It is easily demonstrated that, in such cases, the thickness of the wall layer where the concentration drop occurs is of the order of few times the characteristic length Δy^* , defined as

$$\Delta y^* = \frac{H}{\sqrt{Da}} = \sqrt{\frac{D_{eff}}{\lambda_C}} \quad (25)$$

For intermediate cases, the concentration profiles follow, in the bulk flow, a cosine shape whose extrapolated intersection at $y = H$ depends on S_{min}/S_{max} , while they drop to 0 in the wall region much similarly to

the limiting case (B) (Fig. 2). The thickness Δy^* shows little dependence on S_{min}/S_{max} (except for cases very close to (A)), while mainly depends on physical parameters as described by Eq. (25).

For realistic physical parameters values, Eq. (25) predicts Δy^* values of the order of 10^{-3} m or even less. Despite being strictly valid for simplified problems, these results offer a useful tool to understand the typical behavior of local concentration profiles close to walls also in more realistic cases. As anticipated, steep concentration gradients are therefore expected whenever homogeneous-Dirichlet-like boundary conditions are used in combination with distributed sources which do not vanish in the wall region. Particle deposition calculations in liquid-fuel reactors such as the MSFR fall under such conditions, and are therefore affected by relevant numerical consequences, as described in Section 4, since a grid size of the order of Δy^* or less is needed to correctly resolve the wall layer. We put emphasis on the role which wall gradients - and therefore the ability to resolve them - in determining the flux of deposited particles towards walls. From Eq. (16), the local deposition flux is defined as

$$J_d = -D_{eff} \nabla C \cdot \mathbf{n} \quad (26)$$

and, from a simple steady-state balance, the corresponding surface concentration of deposited particles reads

$$C_d = -\frac{D_{eff}}{\lambda_C} \nabla C \cdot \mathbf{n} \quad (27)$$

4. Applications

The developed solver is tested on two different multiphysics cases. While in (Di Ronco et al., 2021) the implementation was verified against analytical results for a simplified channel geometry problem, here we seek the simulation of full multiphysics cases in more realistic MSFR-related geometries. In the first one, described in Section 4.1, we select a geometry based on the well-known lid-driven square laminar cavity. Even though still fairly simplified, the case features full coupling between thermal–hydraulics and neutronics. Geometry and parameters were chosen for an international benchmark for MSR codes (Tiberga et al., 2020), and this work may represent an extension of the MSFR benchmark towards solid FP simulation. In the second one, described in Section 4.2, a 2D MSFR geometry developed in the EVOL project is used. It features the loop structure typical of the MSFR with fuel recirculation, allowing for the simulation of more realistic turbulent cases. Both cases are selected for their simplified geometric features, which enable the

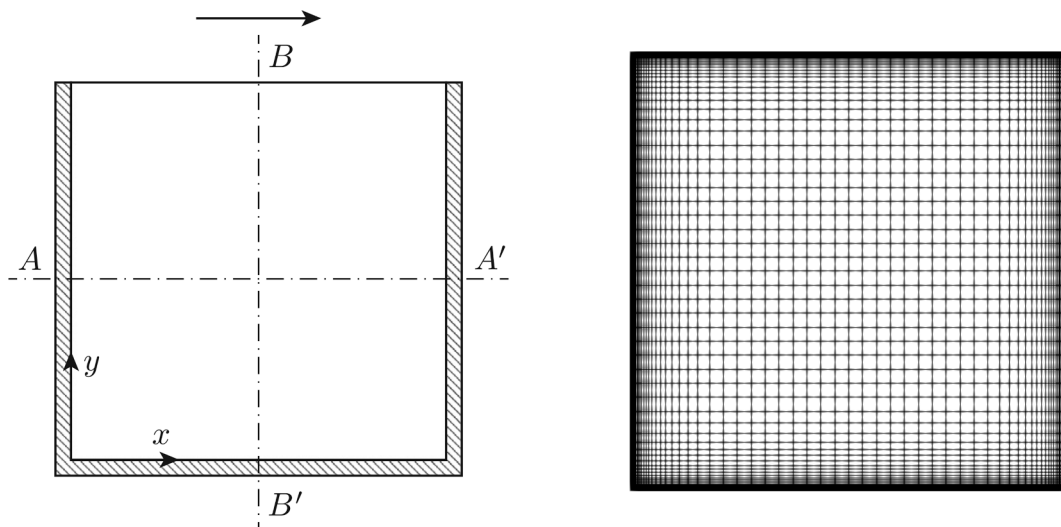


Fig. 3. Lid-driven cavity: geometry (from Tiberga et al. (2020), left) and computational mesh (coarsest case, right). The grid is refined by means of a constant growth-rate in the first 40 layers of cells, starting from a prescribed smallest layer size.

Table 1

Main physical parameter values adopted for the lid-driven cavity case (Tiberga et al., 2020).

Parameter	Symbol	Units	Value
Density	ρ	kg m^{-3}	2.0×10^3
Kinematic viscosity	ν	$\text{m}^2 \text{s}^{-1}$	2.5×10^{-2}
Specific heat capacity	c_p	$\text{J kg}^{-1} \text{K}^{-1}$	3.075×10^3
Thermal expansion coeff.	β_T	K^{-1}	2.0×10^{-4}
Ref. temperature	T_0	K	900
Prandtl number	Pr	–	3.075×10^5
Schmidt number	Sc	–	2.0×10^8
Heat removal coeff.	γ_r	W K^{-1}	4.0×10^6
Heat sink temperature	T_{sink}	K	900

production of high-quality numerical grids even when wall refinement is crucial for the resolution of particle transport in the wall regions, as seen in Section 3. Furthermore, the adoption of 2D cases allows for a significant reduction of computational requirements with respect to full 3D simulations.

The physical properties needed for the simulation of FP particles are kept the same for each case to provide comparable results. The decay constant λ_C has been set to 10^{-5} s^{-1} , which corresponds to a nuclide half-life of approximately one day. The equivalent fission yield y_C has been set to 10^{-2} . Such values are not specific to a particular nuclide, but have been chosen to mimic the behavior of the entire class of noble metal particles.

4.1. Lid-driven cavity

The lid-driven cavity was recently employed to develop a reference case for a numerical benchmark of different multiphysics MSFR codes. A detailed description of the case and of the benchmark procedure can be found in (Tiberga et al., 2020). The domain is characterized by a 2 m by 2 m cavity filled with molten salt (Fig. 3). The domain is treated as a homogeneous, bare reactor. Therefore, standard vacuum conditions are applied for the neutron flux to each boundary, together with a (reflective) homogeneous Neumann condition for the delayed neutron precursors. Decay heat precursors are not simulated in this case, for better consistency with (Tiberga et al., 2020). The driving force for the liquid fuel flow is given by the upper lid, which moves at constant velocity of 0.5 m s^{-1} . All walls are treated as adiabatic, while energy is removed from the system through a simple volumetric heat sink:

$$q_r''' = -\frac{\gamma_r}{V_r}(T - T_{\text{sink}}) \quad (28)$$

where γ_r is a total heat removal coefficient and V_r is the volume of heat removal region, which in this case coincides with the entire cavity domain. The main physical case parameters are summarized in Table 1. Being the analysis conducted in steady-state conditions, simulations are performed in criticality eigenvalue mode with the integrated power normalized to 1000 MW.

With respect to the classic lid-driven case, the coupling with the distributed energy source through buoyancy significantly affects the flow pattern, producing more complex recirculation structures and making this test case suitable for study with multiphysics solvers, despite its overall simplicity.

The computational mesh is produced by specifying a small set of parameters: the number of divisions (equal in both directions), the thickness of the cells in the first boundary layer and the number of cells to be progressively refined. To correctly resolve the concentration boundary layers, a thickness of 10^{-4} m has been chosen according to results of the analytical analysis conducted in Section 3. The resolution of the boundary layer is particularly relevant for the correct prediction of the deposition rates. The prescribed refinement is found to adequately cover the boundary layer with several cell layers. The number of refined cells has been set to 40. For what concerns the number of divisions, three different values have been considered: 100, 200 and 400. Considering the two directions separately, the meshing routine computes a constant cell growth-rate which produces a smooth transition between the refined region and the rest of the domain (where the growth-rate is set to 1). Fig. 3 shows the mesh for the coarsest case (100 divisions).

4.2. EVOL axisymmetric MSFR

A simplified 2D axisymmetric geometry is adopted following the work of the past EVOL project (Brovchenko et al., 2013). Solid parts in the system are neglected as well. The full geometry is shown in Fig. 4, together with some information regarding the position of the heat exchanger and pump sections. The heat exchanger is modeled similarly as in the cavity case, through the use of a linear sink term analogous to Eq. (28). The heat removal coefficient γ_r is here assumed to be zero outside the heat exchanger region. For what concerns the pump, a momentum source is imposed, along the vertical direction, which matches the flow rate at the pump outlet section to the total one ($1.9 \times 10^4 \text{ kg}$

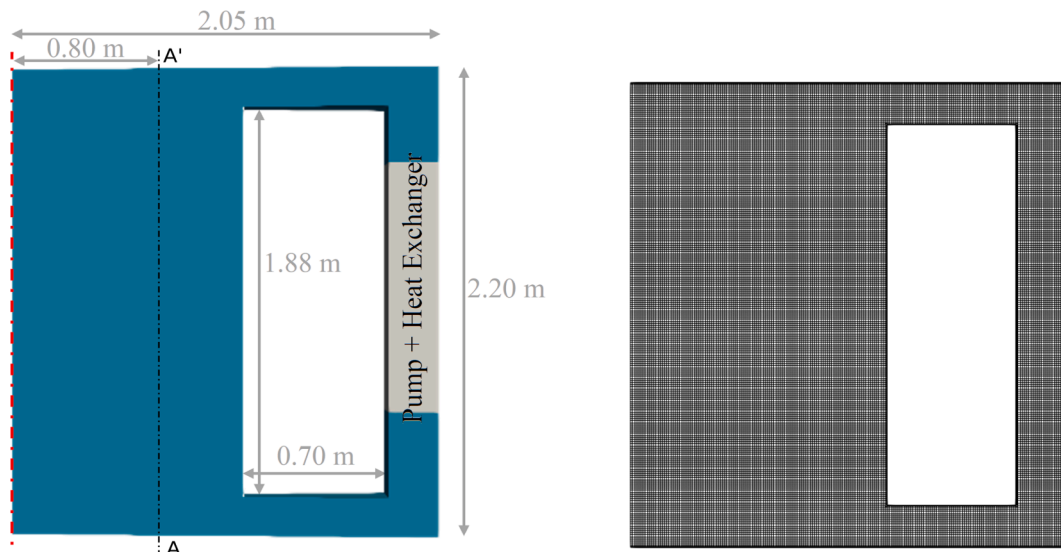


Fig. 4. EVOL case: an axisymmetric geometry (left) is chosen to reduce the computational requirements and the resulting mesh (right) is predominantly structured thanks to the simple geometry employed. Wall mesh refinement is obtained by subsequent divisions of the wall layer.

Table 2
Main physical parameter values adopted for the EVOL case.

Parameter	Symbol	Units	Value
Density	ρ	kg m^{-3}	4.307×10^3
Kinematic viscosity	ν	$\text{m}^2 \text{s}^{-1}$	5.89×10^{-6}
Specific heat capacity	c_p	$\text{J kg}^{-1} \text{K}^{-1}$	1.594×10^3
Thermal expansion coeff.	β_T	K^{-1}	1.912×10^{-4}
Ref. temperature	T_0	K	973
Prandtl number	Pr	–	23.78
Turb. Prandtl number	Pr_t	–	0.85
Schmidt number	Sc	–	20.0
Turb. Schmidt number	Sc_t	–	0.50/0.85/1.20
Heat removal coeff.	γ_r	$\text{W m}^{-2} \text{K}^{-1}$	2.5×10^6
Heat sink temperature	T_{sink}	K	900

s^{-1} , for the entire reactor). The main physical case parameters are summarized in Table 2.

The simplified geometry allows for the production of good-quality structured meshes with little effort. In this case, a cell size of 0.01 m is employed across all the domain for the generation of the underlying mesh (Fig. 4). Then, subsequent cell divisions are applied to the first boundary layer of cells to provide a suitable mesh refinement in the wall region. Boundary layer cells are roughly halved 6 times, to produce a first layer with a thickness of approximately 10^{-4} m. The total number of mesh elements is around 4.2×10^4 .

Three different steady-state cases are simulated to assess the effect of turbulence modeling on the transport of FP particles. As described in Section 2.1, the solver makes use of the standard linear eddy viscosity approach for the modeling of turbulent quantities. The eddy viscosity ν_t affects the transport problem in a direct way, through the definition of the total mass transfer coefficient D_{eff} , and through the computation of the velocity field. For this reason, three different turbulence models are used: standard $k-\epsilon$ (Lauder and Spalding, 1974), the standard $k-\omega$ (Wilcox, 2008) and the $k-\omega$ -SST (Menter, 1994). Gradient-based turbulent diffusion constitutes a standard approach in CFD and multiphysics analysis, but relies heavily on the turbulent Schmidt number Sc_t , with optimal values depending on fluid properties and on flow configuration (Tominaga and Stathopoulos, 2007). Given the lack of experimental data for MSFR applications, in this work we select three different values (0.50, 0.85 and 1.20) to provide insight on the influence of such parameter on simulations over a relatively broad range of variation.

5. Results and discussion

5.1. Lid-driven cavity

Steady-state simulations have been performed with the three different mesh refinements described earlier. These preliminary laminar simulations have been conducted to study the effects of grid refinement. We stress that an adequate refinement is crucial for the prediction of deposition rates. For reference, velocity and temperature distributions are shown in Fig. 5. As anticipated, the interplay between the upper lid motion and the buoyancy effects produces complex recirculation patterns with two separate large laminar eddies, in contrast with the classical isothermal lid-driven cavity problem.

Concentration results for the different mesh refinements are reproduced in Fig. 6 and in Fig. 7 for what concerns distributions in the domain and profiles in the wall layers close to left and right walls, respectively. While the wall refinement guarantees a proper resolution of the wall layers in all cases, showing a suitable number of grid points even in the coarsest case thanks to the specific meshing procedure adopted which specifies the thickness of the first layer, only the most refined grid is able to capture all transport patterns in the domain. One possible cause is due to the use of gradient-limited upwind-biased 2nd-order divergence schemes. While 2nd-order schemes are needed to ensure proper accuracy, their use with low-quality meshes is known to produce poor results. On the other hand, the nature of the problem forces the use of upwind-biased schemes to provide a good balance between stability and accuracy, while gradient limiting is needed to ensure boundedness in the presence of steep gradients such as the ones which occur in the wall layers. Other transported quantities, such as neutron precursors, do not need this kind of numerical treatment due to the different reflective boundary conditions adopted.

Wall concentration profiles are characterized by different “asymptotic values” depending on the grid refinement and the overall accuracy dictated by the quality of the mesh. Nevertheless, within the wall layer, concentration profiles exhibit similar behavior, somewhat confirming some of the results given by the analytical treatment of Section 3. Using the values specified for λ_C, ν and Sc , Eq. (25) predicts a value for Δy^* of about 0.0035 m. Even though the mesh refinement has been selected to ensure fairly thinner boundary elements, such value is not found to be sufficiently representative of the results from Fig. 7. Computed profiles show significantly thinner wall layers, suggesting a strong influence of

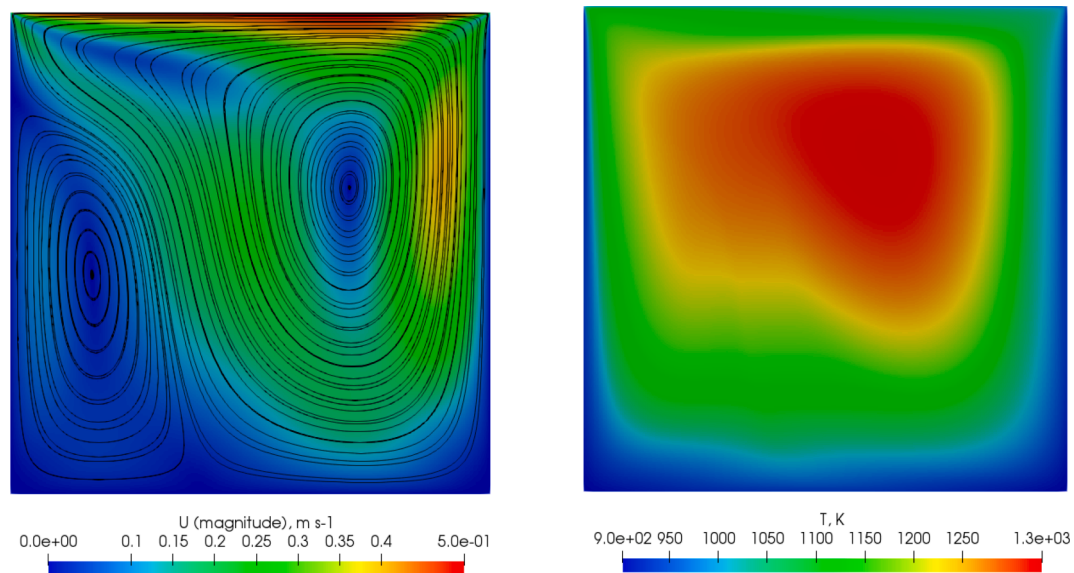


Fig. 5. Velocity U (left) and temperature T (right) distributions in the lid-driven cavity (most refined mesh, 400 divisions). Velocity streamlines are also added for more clarity. The combined action of lid motion and buoyancy affects the flow pattern, producing two separate recirculation zones.

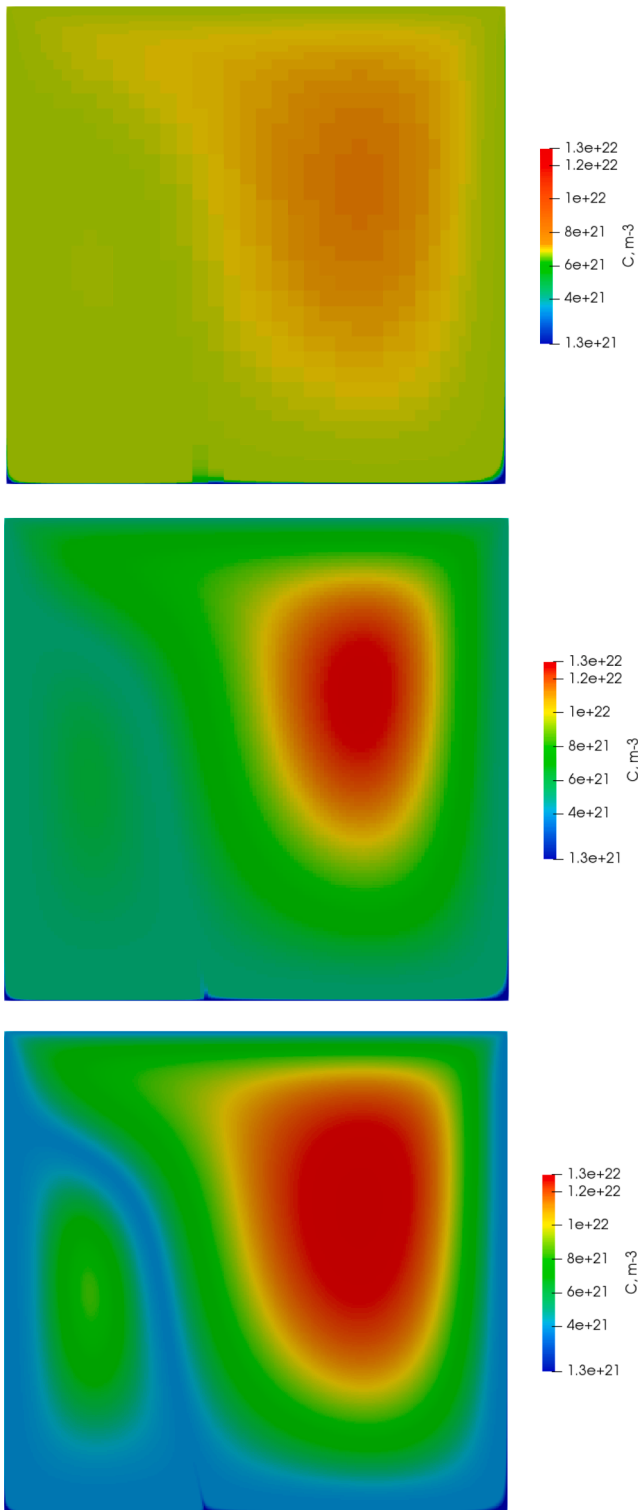


Fig. 6. Particle concentration C distributions for three different mesh refinements: from top to bottom, 100, 200, and 400 divisions in both directions.

local velocity patterns and transport mechanism with respect to the simplified approach adopted in the analytical model. This is particularly evident from the comparison between the left and right walls, where the right wall layer is approximately 3–4 times larger than the left one. Nevertheless, the analytical treatment proves a useful tool to predict estimates and to understand the role of the main physical parameters.

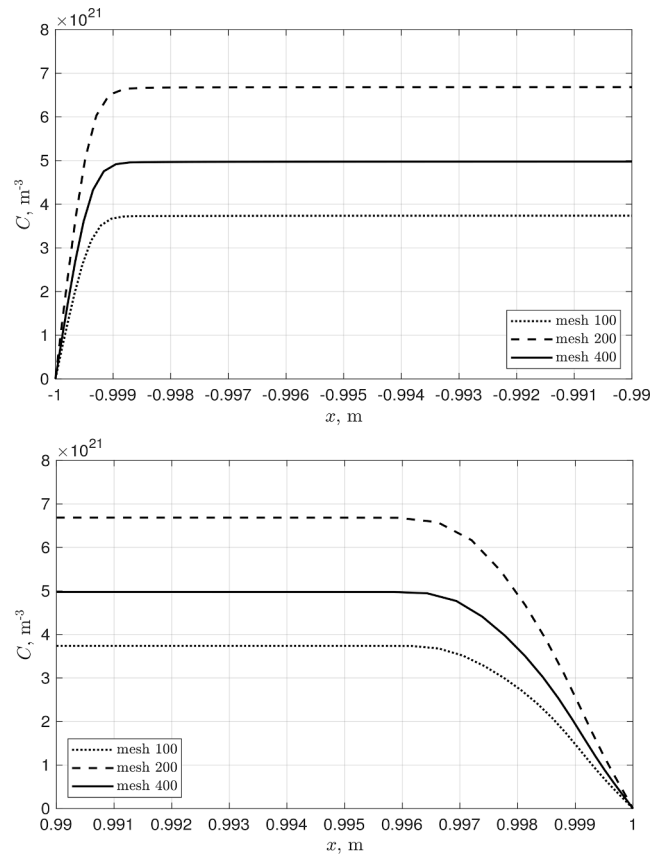


Fig. 7. Particle concentration C wall profiles for three different mesh refinements. Line plots correspond to a horizontal line at half the cavity height on the left (top plot) and right (bottom plot) walls, corresponding to points A and A' of Fig. 3.

5.2. EVOL axisymmetric MSFR

Steady-state simulations have been conducted with the selected turbulence models and values for Sc_t for a total of nine cases, as described earlier. As in the cavity cases, 2nd-order upwind-biased gradient-limited convergence schemes have been used for the simulation of FPs. For reference, velocity and total kinetic viscosity distributions are shown in Fig. 8. As expected, the choice of turbulence model has an evident impact on the prediction of U and ν_{eff} , in particular when comparing turbulence models from the $k-\epsilon$ and $k-\omega$ families. Such differences have a direct influence on the combined effect of advective and diffusive transport mechanisms for FPs, as better evidenced by Fig. 9, which shows the volume distributions of the particle concentration C for the three simulated cases. Maximum and average particle concentrations are approximately one order of magnitude lower in the $k-\epsilon$ case than in the other cases, qualitatively in accordance with the higher $k-\epsilon$ diffusivity.

The same behavior is observed, naturally, in the concentration profiles close to walls. Fig. 10 shows concentration profiles close to the bottom and top walls, in correspondence of a vertical line placed at 0.8 m from the reactor symmetry axis (Fig. 4). Also in this case, gradient limiting allows for the computation of steep wall gradients without the insurgence of instability issues, while the prescribed mesh refinement proves adequate to resolve correctly the gradients. Once again, the thickness of the wall layers shows values of the order of 10^{-3} m, which clearly demonstrates the importance of local velocity profiles and of turbulence in determining the steepness of the concentration gradients and thus the required grid refinement in the wall regions. It appears evident that also the choice of turbulence model itself affects to some

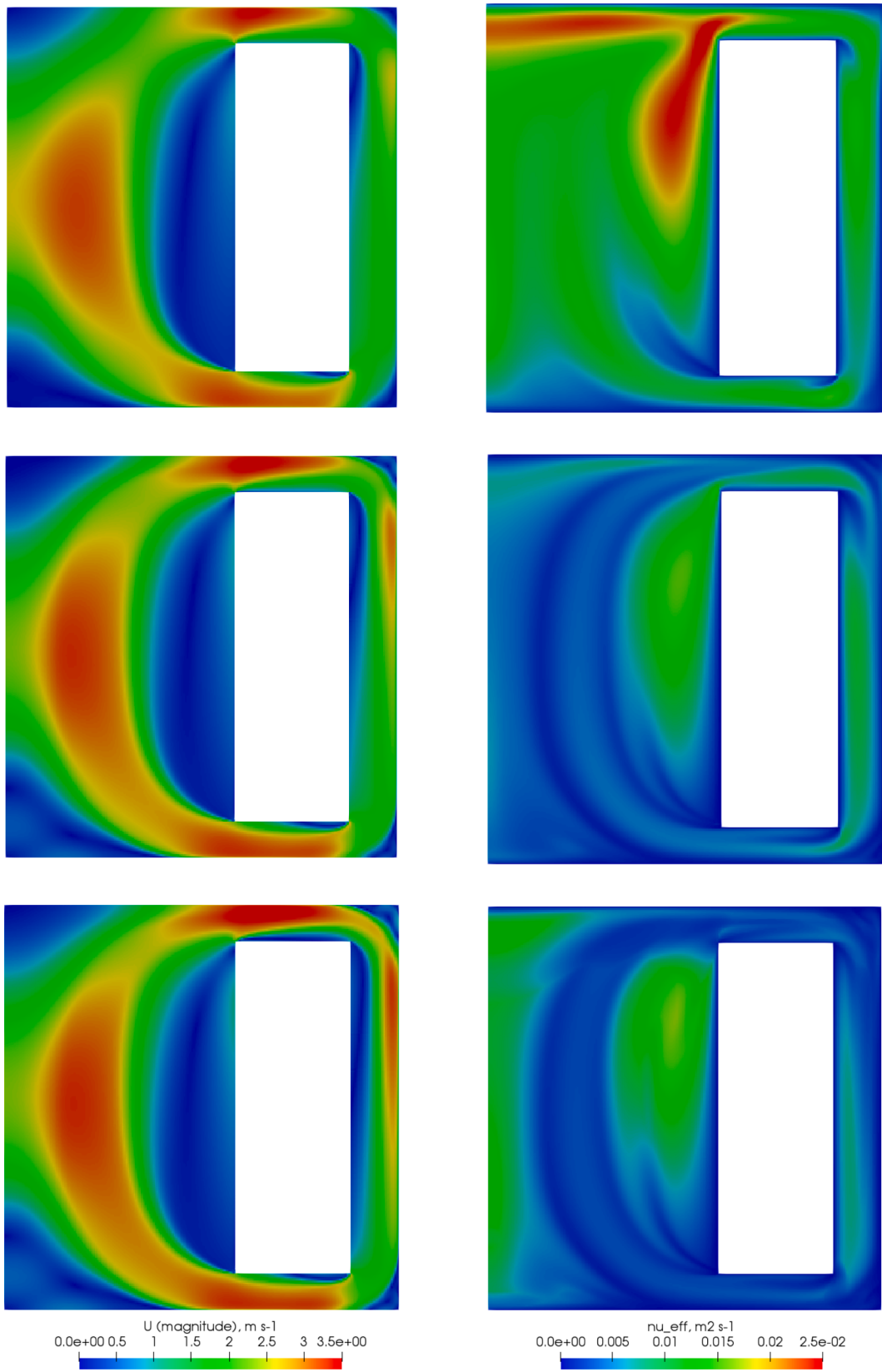


Fig. 8. Magnitude of velocity u (left) and total kinetic viscosity ν_{eff} (right) distributions in the EVOL reactor for the $k-\epsilon$, $k-\omega$ and $k-\omega-SST$ turbulence models (from top to bottom).

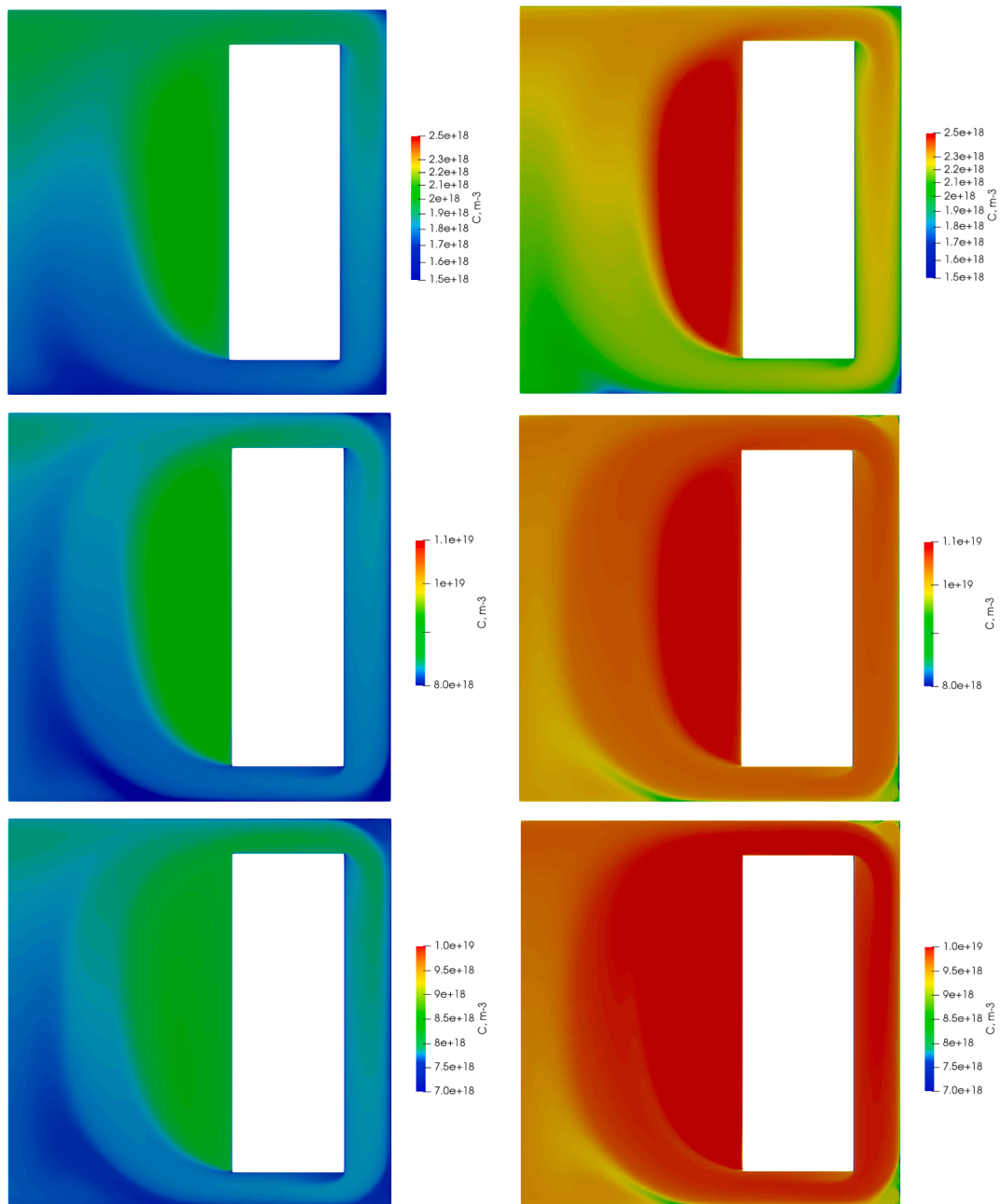


Fig. 9. Particle concentration C distributions for the $k-\varepsilon$, $k-\omega$ and $k-\omega-SST$ turbulence models (from top to bottom). Plots on the left and right columns refer to Sc_t equal to 0.50 and 1.20, respectively.

degree the thickness of the wall layers. Nevertheless, also in this case the thickness values predicted by the analytical model have proven useful, at least as preliminary estimates.

The integrated deposited fraction, together with other integral information are reported in Table 3. It appears from the results that, besides the differences in the total number of precipitate particles between the three cases, the choice of the turbulence model has a very limited influence on the number of deposited particles. This is a direct consequence of the similar gradients computed by the three models. Furthermore, in the diffusive wall layers the eddy diffusivity tends to zero and therefore the total value tends to the laminar one ($\nu/Sc = 2.945 \cdot 10^{-7} \text{ m}^2 \text{ s}^{-1}$), which is the same for the three cases.

The choice of the turbulent Schmidt number appears to play a similar role: larger values lead to lower diffusivities and increased precipitate concentrations, but deposition rates are scarcely affected. This confirms

the prevalence of laminar diffusion in transport mechanisms close to walls, as shown by the similar wall concentration profiles shown in Fig. 10, and allows for a certain flexibility in the choice of Sc_t as far as deposition figures are concerned. Lastly, the transport mechanisms towards the walls appear efficient when compared to the intensity of radioactive decay (in our cases, $\lambda_C = 10^{-5} \text{ s}^{-1}$), since more than 99.9% of particles end up depositing on walls. This effect is expected to be even more significant for longer-lived metallic FPs.

6. Conclusions

In this paper, previously developed transport models for the solid fission products in the MSFR have been tested on two separate molten salt cases, namely the lid-driven cavity problem and the EVOL geometry. The employed models are based on a Eulerian single-phase framework,

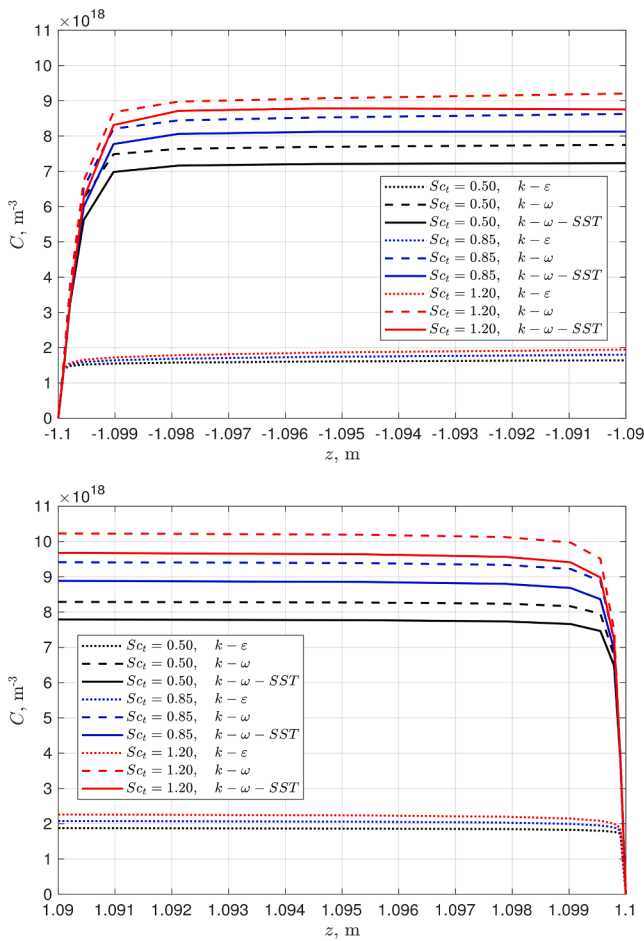


Fig. 10. Particle concentration C wall profiles for different values of the turbulent Schmidt number Sc_t and turbulence models. Line plots correspond to vertical lines of length 0.01 m placed at 0.8 m from the reactor symmetry axis from the bottom (top plot) and top (bottom plot) walls (see points A and A' of Fig. 4).

implemented in a consolidated MSFR multiphysics solver based on the open-source finite-volume library OpenFOAM. The main subjects of the investigation were the prediction of particle deposition fluxes and the analysis of related numerical issues arising from the commonly adopted assumption of “perfectly adsorbing” walls in combination with distributed particles source. The influence of different turbulence modeling approaches and turbulent diffusion parameters on particle distributions and deposition fluxes was also tested in the EVOL case.

Analytical results based on a simplified laminar parallel-plates geometry have been used to determine the expected particle concentration gradients close to solid walls. It was observed that the interplay between homogeneous Dirichlet boundary conditions and the presence of a non-negligible particle source in the wall layers produces steep gradients, and therefore poses the need for significant mesh refinement in the wall regions. Furthermore, the presence of steep gradients and the need to correctly resolve the boundary layers require, besides an adequate mesh refinement, the adoption of second order discretization schemes combined with gradient limiting to avoid numerical instability. Wall layer thicknesses in both the cavity and EVOL cases have not been found in complete agreement with the analytical estimate, demonstrating the role of geometry, local velocity profiles and of turbulence. However, prescribed mesh refinement based on the analytical model proved sufficient to adequately resolve wall concentration gradients in all simulated cases. The comparison of three different common turbulence models, namely the standard $k-\epsilon$, the standard $k-\omega$ and the $k-\omega-SST$

Table 3

EVOL case: main simulation results for the selected turbulence models and values of Sc_t . The balance error is computed as the relative difference between the integral source and the sum of the integral deposition and decay rates.

Quantity	Units	$k-\epsilon$	$k-\omega$	$k-\omega-SST$
$Sc_t = 0.50$				
Total precipitate	–	4.8516678×10^{17}	2.1769658×10^{18}	2.0492698×10^{18}
Total deposit	–	1.2627549×10^{21}	1.2610617×10^{21}	1.2611896×10^{21}
Total source	s^{-1}	1.2632382×10^{16}	1.2632367×10^{16}	1.2632370×10^{16}
Total deposition rate	s^{-1}	1.2627549×10^{16}	1.2610617×10^{16}	1.2611896×10^{16}
Total decay rate	s^{-1}	4.8516678×10^{12}	2.1769658×10^{13}	2.0492698×10^{13}
Rel. balance error	–	$-1.5241115 \times 10^{-6}$	$-1.5441926 \times 10^{-6}$	$-1.5458692 \times 10^{-6}$
$Sc_t = 0.85$				
Total precipitate	–	5.4409856×10^{17}	2.4950726×10^{18}	2.3620182×10^{18}
Total deposit	–	1.2626960×10^{21}	1.2607436×10^{21}	1.2608769×10^{21}
Total source	s^{-1}	1.2632381×10^{16}	1.2632367×10^{16}	1.2632370×10^{16}
Total deposition rate	s^{-1}	1.2626960×10^{16}	1.2607436×10^{16}	1.2608769×10^{16}
Total decay rate	s^{-1}	5.4409856×10^{12}	2.4950726×10^{13}	2.3620182×10^{13}
Rel. balance error	–	$-1.5586352 \times 10^{-6}$	$-1.5458756 \times 10^{-6}$	$-1.5454547 \times 10^{-6}$
$Sc_t = 1.20$				
Total precipitate	–	5.9885298×10^{17}	2.7344317×10^{18}	2.5986233×10^{18}
Total deposit	–	1.2626413×10^{21}	1.2605042×10^{21}	1.2606403×10^{21}
Total source	s^{-1}	1.2632382×10^{16}	1.2632367×10^{16}	1.2632370×10^{16}
Total deposition rate	s^{-1}	1.2626413×10^{16}	1.2605042×10^{16}	1.2606403×10^{16}
Total decay rate	s^{-1}	5.9885298×10^{12}	2.7344317×10^{13}	2.5986233×10^{13}
Rel. balance error	–	$-1.5255000 \times 10^{-6}$	$-1.5445096 \times 10^{-6}$	$-1.5561749 \times 10^{-6}$

models, with different turbulent Schmidt number values has shown a significant influence on the particle concentration distributions, given the discrepancies in the predicted velocity and eddy diffusivity fields. However, the deposition rates, which are one of the main subjects of the analysis, were much less affected, suggesting a certain flexibility in the choice of turbulence models and parameters as far as deposition is concerned. This effect is probably due to the fact that, in the concentration boundary layer, transport is dominated by diffusion and turbulent diffusivity tends to zero at walls. In connection with this aspect, it was found that, in steady-state conditions, a large fraction (more than 99.9%) of particles borne in the fuel are found on walls, demonstrating the efficiency of transport mechanisms within the reactor. This aspect might prove even more relevant when long-lived metallic species are considered, given the competition between the deposition and decay mechanisms in determining the fate of produced particles.

Despite relevant for the analysis of MSFR behavior, the adopted geometries were selected to simplify the numerical analysis and to reduce the computational requirements. Future work will include the analysis of FPs transport in a more realistic 3D reactor simulation. The study of the EVOL case has shown that the effect of turbulent transport in relatively complex geometries should not affect dramatically concentration gradients close to walls, giving reasonable estimates of the

required mesh refinement. Arbitrary and flexible mesh refinement in more complex 3D geometries, however, may prove a challenging task. Other possible extensions of the present work might include the adoption of more sophisticated turbulence modeling approaches such as Large Eddy Simulation. In this perspective, it is worth noting that preliminary work suggested that 3D models, especially following a LES approach, should require a significant increase in the cell count (above 10^6), with a computational cost in the range of several thousands CPU-hours for transients of a few tens of seconds. Regarding other limitations of the multiphysics transport model, the integration with a (possibly simplified) chemistry model to distinguish between the solid and the dissolved species might further improve the descriptive capabilities of the multiphysics tool. Finally, the effects of particles size on transport need to be addressed. Therefore, future developments should focus on such problem, possibly by considering the adoption of more sophisticated modeling approaches to take particle growth and inertial effects into account.

Data availability statement

The data that support the findings of this study are openly available in Zenodo at <http://doi.org/10.5281/zenodo.5541560>.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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