# Species Tracking

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# Adding two-phase flow modeling to thermal-hydraulics model
## *Pronghorn's two-phase mixture model*

The mixture continuity equation:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \bar{v}_m / \gamma) = 0$$

The continuity equation for phase 2:

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot (\alpha_2 \rho_2 \bar{v}_m / \gamma) = \Gamma_2 - \nabla \cdot \left( \frac{\alpha_2 \rho_1 \rho_2}{\rho_m} \bar{v}_{slip,d} \right)$$

The mixture momentum equation:

$$\frac{\partial}{\partial t} \rho_m \bar{v}_m + \nabla \cdot (\rho_m \bar{v}_m \bar{v}_m / \gamma) = -\nabla \gamma p_m + \nabla \cdot (\alpha_1 \mu_1 + \alpha_2 \mu_2) \nabla \bar{v}_m - \nabla \cdot \left( \frac{\alpha_2}{1 - \alpha_2} \frac{\rho_1 \rho_2}{\rho_m} \bar{v}_{slip,d} \bar{v}_{slip,d} / \gamma \right) + \gamma \rho_m g_m + \gamma M_m$$

The slip velocity is modeled as

$$\bar{v}_{slip,d} = \frac{\tau_d}{f_{drag}} \frac{\rho_d - \rho_m}{\rho_d} \bar{a}$$

where:

- $\tau_d$ is the particle relaxation time, $f_{drag}$ is the linear drag coefficient function, $\rho_d$ is the density of the dispersed phase, $\bar{a}$ is the acceleration vector.

The particle relaxation time is modeled as follows Bilicki and Kestin (1990):

$$\tau_d = \frac{\rho_d d_d^2}{18 \mu_m}$$

where:

- $d_d$ is the particle diameter, $\mu_m$ is the mixture dynamic viscosity.

The acceleration vector is the particle acceleration vector:

$$\bar{a} = \bar{g} + \frac{\bar{f}}{\rho_m} - \bar{u}_m \cdot \nabla \bar{u}_m - \frac{\partial \bar{u}_m}{\partial t}$$

where:

- $\bar{f}$ is the volumetric force

# Adding two phase flow to thermal-hydraulics

Adding Void Fraction Solution Variable

```
[void_f]
  type = INSFVScalarFieldVariable
  initial_from_file_var = void_f
  block = ${fluid_blocks}
[]
```

Adding Void Fraction Kernels

```
[void_f_time]
  type = FVFunctorTimeKernel
  variable = void_f
  block = ${fluid_blocks}
[]
[void_f_advection]
  type = INSFVScalarFieldAdvection
  variable = void_f
  u_slip = 'superficial_vel_slip_x'
  v_slip = 'superficial_vel_slip_y'
  block = ${fluid_blocks}
[]
[vod_f_diffusion]
  type = INSFVMixingLengthScalarDiffusion
  schmidt_number = '${fparse Sc_t/10.0}'
  variable = void_f
  block = ${fluid_blocks}
[]
[void_f_src]
  type = FVCoupledForce
  variable = void_f
  v = fission_source
  coef = ${gas_fraction}
[]
[void_f_sink_pump]
  type = NSFVEnergyAmbientConvection
  variable = void_f
  T_ambient = 0.0
  alpha = 100.0
  block = 'pump'
[]
```

Time Derivative

Advection via Slip Velocity

Turbulent Diffusion

Void Source due to Nuclear Fission

Void Sink at Pump due to Gas Removal

# Defining mixture properties materials

```
[mixing_material]
  type = NSFVMixtureFunctorMaterial
  phase_1_names = 'rho mu'
  phase_2_names = '${rho_d} ${mu_d}'
  prop_names = 'rho_mixture mu_mixture'
  phase_1_fraction = 'phase_1'
  output_properties = 'rho_mixture mu_mixture'
  block = ${fluid_blocks}
[]
```

Defines mixture properties for density and viscosity as a function of the liquid fraction

Compute the arithmetic mean of material properties using a phase fraction.

This material is mainly used in multiphase modeling. Given a phase fraction functor "phase_1_fraction" ($\lambda_1$) and two vectors of (functor) properties "phase_1_names" and "phase_2_names", named generically $p_{i,1}$ and $p_{i,2}$, respectively, the material computes the phase-weighted average of the property as follows:

$$p_i = \lambda_1 p_{i,1} + (1 - \lambda_1) p_{i,2} \, ,$$

From:
https://mooseframework.inl.gov/source/functormaterials/NSFVMixtureFunctorMaterial.html

# Defining slip velocities (drift flux formulation)

```
[populate_u_slip]
  type = WCNSFV2PSlipVelocityFunctorMaterial
  slip_velocity_name = 'superficial_vel_slip_x_no_porous'
  momentum_component = 'x'
  u = superficial_vel_x
  v = superficial_vel_y
  rho = 'rho_mixture'
  mu = 'mu_mixture'
  rho_d = ${rho_d}
  particle_diameter = ${dp}
  block = ${fluid_blocks}
  linear_coef_name = 100.0
[]
[populate_v_slip]
  type = WCNSFV2PSlipVelocityFunctorMaterial
  slip_velocity_name = 'superficial_vel_slip_y_no_porous'
  momentum_component = 'y'
  u = superficial_vel_x
  v = superficial_vel_y
  rho = 'rho_mixture'
  mu = 'mu_mixture'
  rho_d = ${rho_d}
  particle_diameter = ${dp}
  block = ${fluid_blocks}
  linear_coef_name = 100.0
[]
```

Defines slip velocity in the ‘x’ direction

Defines slip velocity in the ‘y’ direction

# Defining interface area concentration

```
[interface_area_concentration]
  type = ADParsedFunctorMaterial
  expression = 'void_f * 6 / ${dp}'
  functor_names = 'void_f'
  functor_symbols = 'void_f'
  property_name = 'interface_area_concentration'
[]
```

Defines interface area concentration

1) $\chi_g = \frac{A_{lg}}{V}$

2) $A_g = n_b 4\pi R^2$

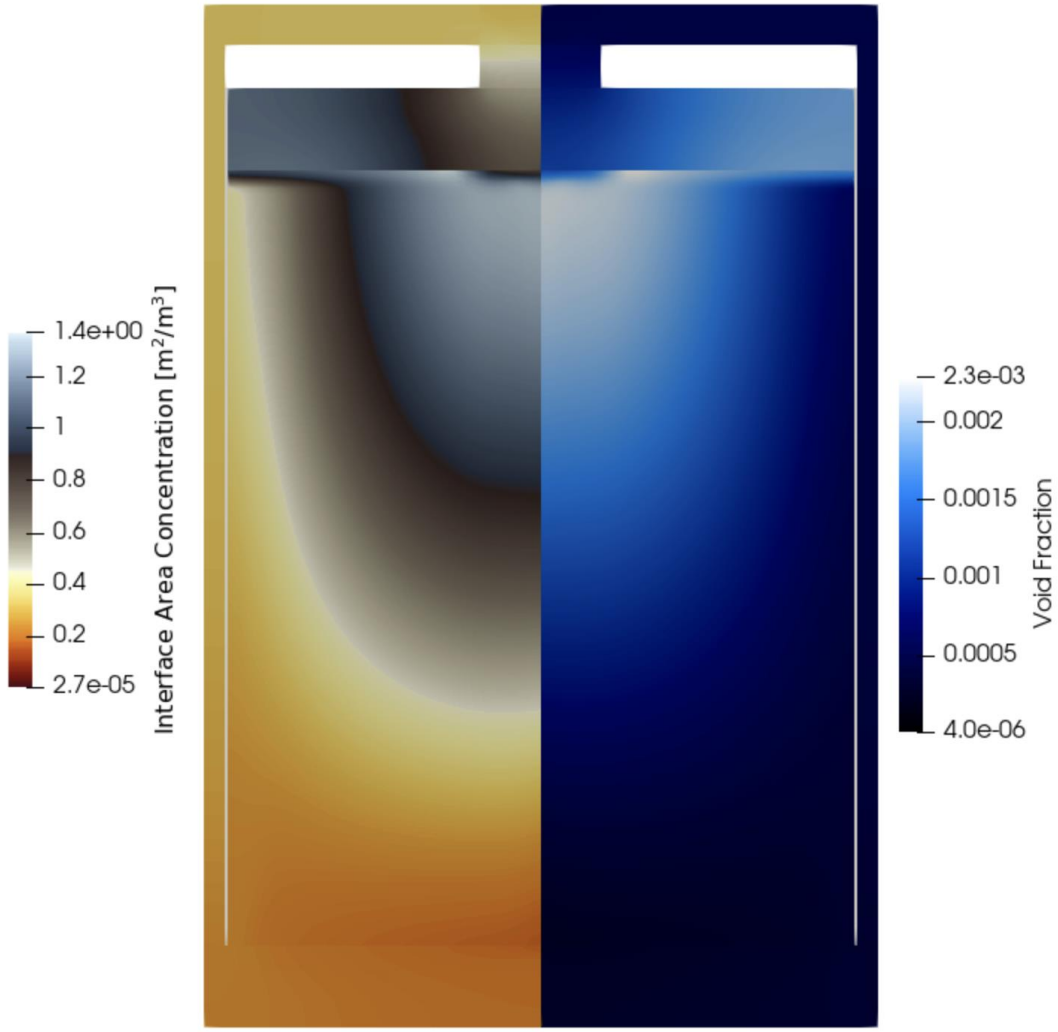
3) $\alpha_g = \frac{V_g}{V} = \frac{1}{V}\, n_b \frac{4}{3}\pi R^3 \rightarrow V = \frac{1}{\alpha_g}\, n_b\, \frac{4}{3}\pi R^3$

2 and 3 into 1) $\chi_g = \alpha_g \frac{n_b 4\pi R^2}{n_b \frac{4}{3}\pi R^3} = \alpha_g \frac{3}{R} = \alpha_g \frac{6}{D_p}$

```
# Average bubble diameter
dp = 0.01
```

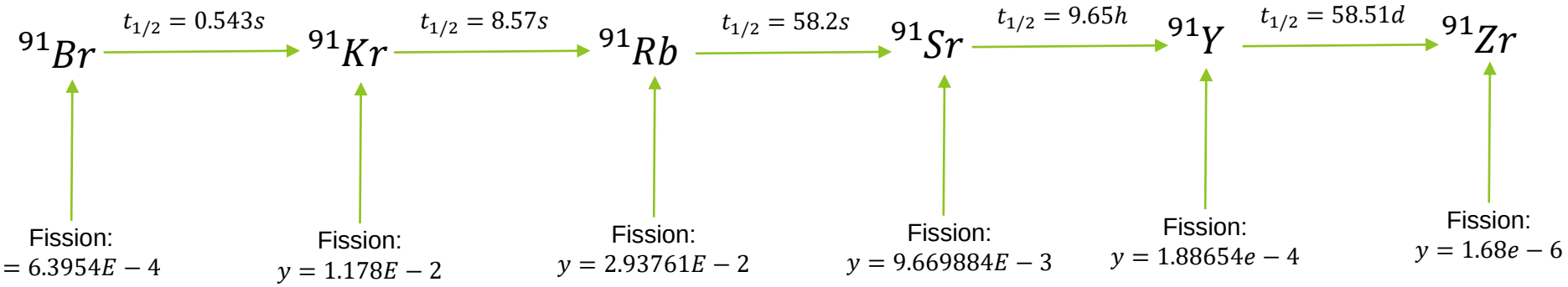
# Steady-state void distribution

- Void increases as the fuel circulate through the reactor core
- As flow mixes in the upper plenum two different behaviors are observed:
  - Flow jets to the riser, where void is removed at the pump
  - Flows is more occluded towards the external radius of the upper plenum, resulting on a higher void concentration
- Interface area concentration and hence, liquid-gas exchange processes are larger at the top of the core and the partially occluded flow in the outer radius of the upper plenum



# Species Tracking
# Example tracking the $^{91}Br$ depletion chain

- The depletion chain for  reads as follows:




- In practice, these reactions happen while species are transported in the fluid. We solve the following equation for isotope concentration $c_i^x$ for isotope $i$ in state $x$:

$$\frac{\partial c_i^x}{\partial t} + \nabla \cdot \left(\frac{\boldsymbol{u}}{\gamma} c_i^x\right) - \nabla \cdot \left[\left(D_{c_i} + \frac{\nu_t}{Sc_t}\right)\nabla c_i^x\right] = y_i f - \lambda c_i^x + h^{xy}(c_i^y - c_i^x)$$

Time derivative | Convection in Porous Media | Molecular and Turbulent Diffusion | Fission Yield Source | Natural Decay Sink | Exchange of phases between states y and x

# Defining the solution variables

```
[Variables]
  [Br91_f]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Br91_g]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Kr91_f]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Kr91_g]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Rb91_f]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Rb91_g]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
  [Sr91_f]
    type = MooseVariableFVReal
    block = ${fluid_blocks}
  []
```

For each of the tracked isotopes, solution variables are defined in the liquid (dissolved) and gaseous states

# Defining the solution kernels
# Example $^{91}Kr$

```
[Kr91_time]
  type = FVFunctorTimeKernel
  variable = 'Kr91_f'
  block = ${fluid_blocks}
[]
[Kr91_advection]
  type = PINSFVMassAdvection
  variable = 'Kr91_f'
  rho = 'Kr91_porous'
  block = ${fluid_blocks}
[]
[Kr91_diffusion]
  type = FVDiffusion
  variable = 'Kr91_f'
  coeff = ${D_mu}
  block = ${fluid_blocks}
[]
[Kr91_turb_diffusion]
  type = INSFVMixingLengthScalarDiffusion
  variable = 'Kr91_f'
  schmidt_number = ${Sc_t}
  block = ${fluid_blocks}
[]
[Kr91_src]
  type = FVCoupledForce
  variable = 'Kr91_f'
  v = fission_source
  coef = ${yield_Kr91}
  block = ${fluid_blocks}
[]
[Kr91_decay]
  type = FVReaction
  variable = 'Kr91_f'
  rate = ${lambda_Kr91}
  block = ${fluid_blocks}
[]
[Kr91_grow]
  type = FVCoupledForce
  variable = 'Kr91_f'
  v = 'Br91_f'
  coef = ${lambda_Br91}
  block = ${fluid_blocks}
[]
[Kr91_fg]
  type = NSFVMixturePhaseInterface
  variable = 'Kr91_f'
  phase_coupled = 'Kr91_g'
  alpha = 'hlg_Kr91'
[]
```

Time derivative

Porous media advection

Molecular diffusion

Turbulent diffusion

Fission source

Natural decay

Buildup due to $^{91}Br$

Fluid-to-gas exchange

```
[Kr91_gf]
  type = NSFVMixturePhaseInterface
  variable = 'Kr91_g'
  phase_coupled = 'Kr91_f'
  alpha = 'hlg_Kr91'
[]
[Kr91_g_advection]
  type = PINSFVMassAdvection
  variable = 'Kr91_g'
  rho = 'Kr91_g'
  block = ${fluid_blocks}
[]
[Kr91_g_diffusion]
  type = FVDiffusion
  variable = 'Kr91_g'
  coeff = ${D_mu_g}
  block = ${fluid_blocks}
[]
[Kr91_g_decay]
  type = FVReaction
  variable = 'Kr91_g'
  rate = ${lambda_Kr91}
  block = ${fluid_blocks}
[]
[Kr91_grow_g]
  type = FVCoupledForce
  variable = 'Kr91_g'
  v = 'Br91_g'
  coef = ${lambda_Br91}
  block = ${fluid_blocks}
[]
```

Gas-to-fluid exchange

Advection is porous media

Molecular gas diffusion

Natural decay

Growth due to decay of $^{91}Br$ in the gas phase

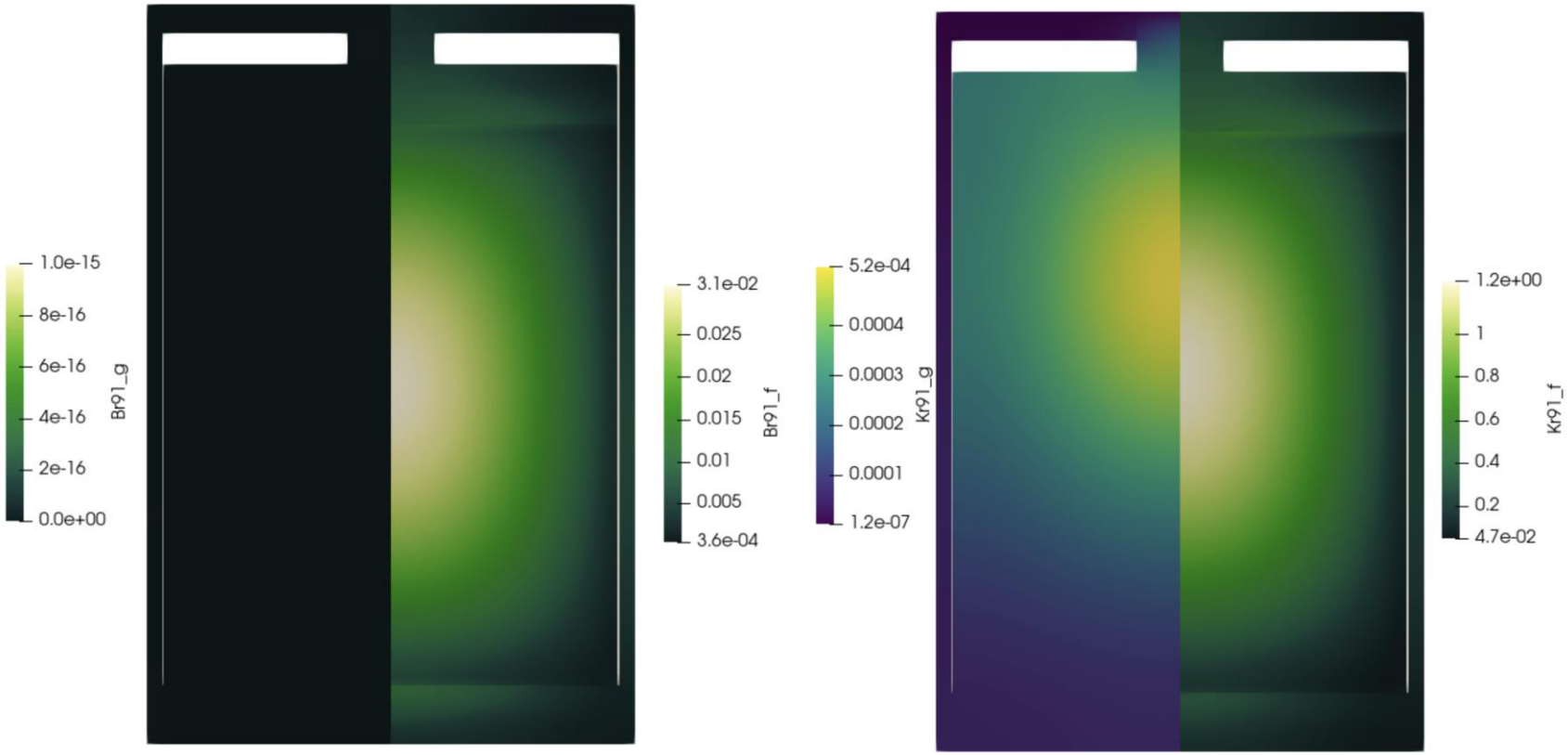
# Liquid-gas exchange coefficients

```
[hlg_Kr91]
  type = ADParsedFunctorMaterial
  expression = 'interface_area_concentration * ${Kr91_alpha_fg}'
  functor_names = 'interface_area_concentration'
  functor_symbols = 'interface_area_concentration'
  property_name = 'hlg_Kr91'
[]
```

For every species, the net volumetric mass exchange coefficient is defined as the surface-specific mass exchange coefficient multiplied by the interface area concentration

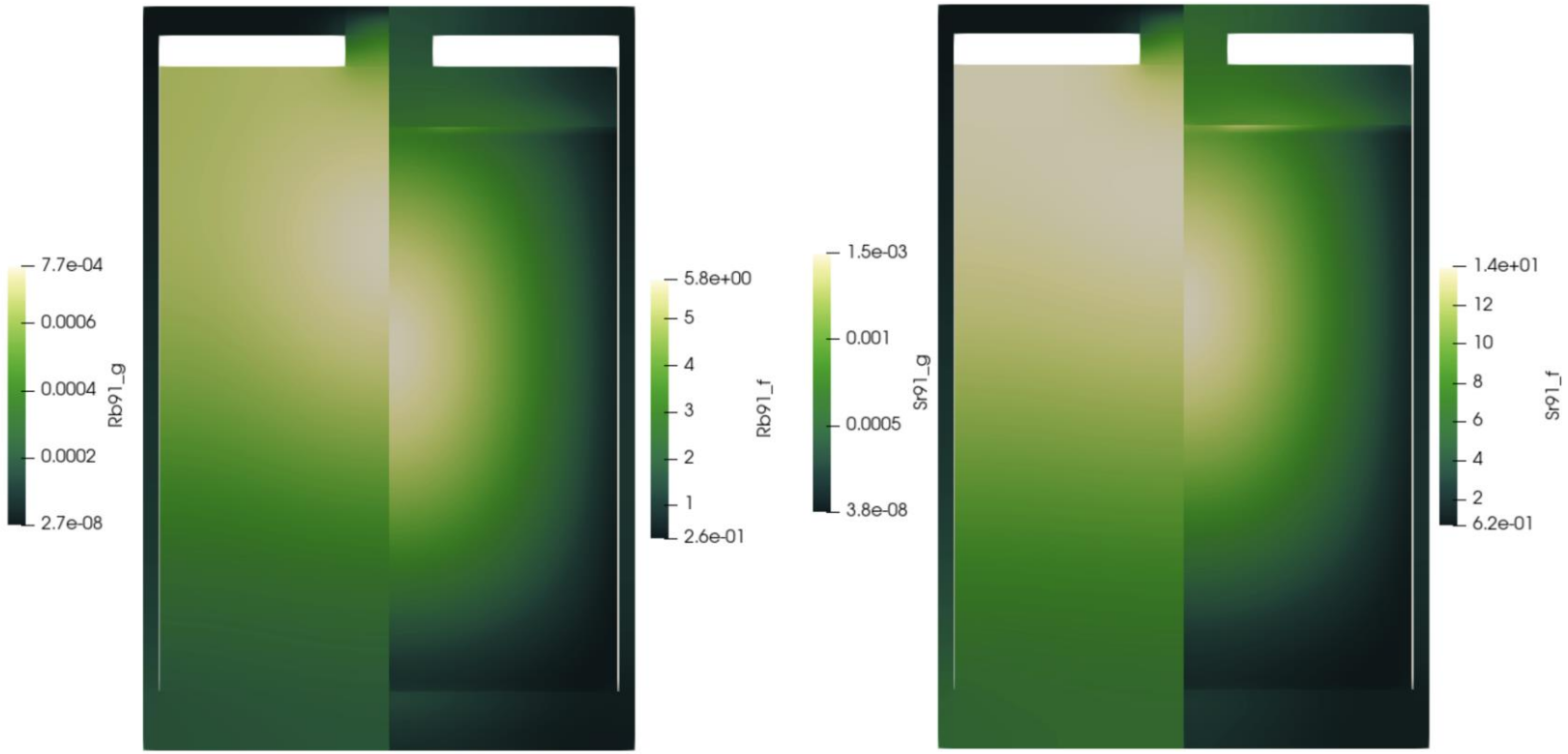
# Simulation Results 1/3

- $^{91}Br$ is produced by fission and stays in solution in the fuel salt
- No gaseous $^{91}Br$ is present
- $^{91}Kr$ is produced by fission and by natural decay of $^{91}Br$ in the fuel salt
- Some $^{91}Kr$ converts into the gas phase, where is transported toward the extraction point at the top of the reactor core



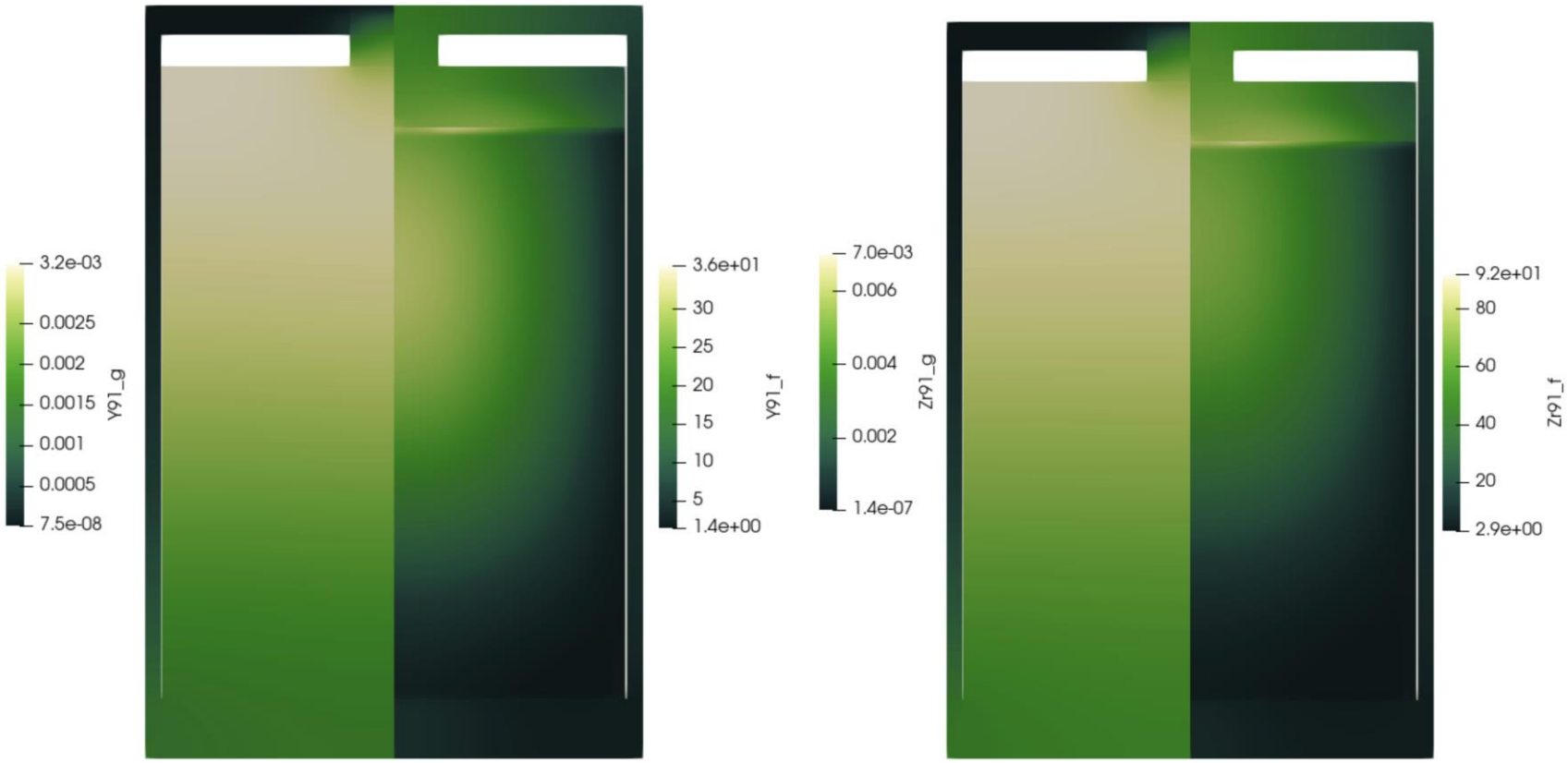
# Simulation Results 2/3

- $^{91}Rb$ is produced by fission and by the decay of $^{91}Kr$ in the fuel salt
- Also, $^{91}Rb$ is produced by the decay of $^{91}Kr$ in the gas phase
- A similar behavior is observed for $^{91}Sr$



# Simulation Results 3/3

- $^{91}Y$ is produced by fission and by the decay of $^{91}Sr$ in the fuel salt
- There is no direct exchange between the liquid and the gas phase for $^{91}Y$
- Also, $^{91}Y$ is produced by the decay of $^{91}Sr$ in the gas phase
- A similar behavior is observed for $^{91}Zr$

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