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International RELAP5 Users Group Meeting And Training Seminars

Improvements to PHISICS/RELAP5-3D© Capabilities for Simulating HTGRs – NK Adaptive time step implementation

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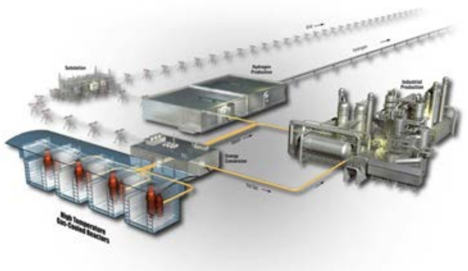
- The objective
- Code & models
- Decoupling scheme
- Adaptive time step
- Conclusions

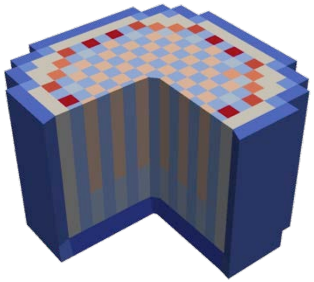
The Objective

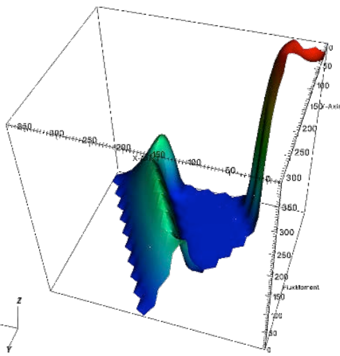
- Improvement of the **PHISICS**/**RELAP5-3D©** coupling scheme to allow the NK code to use a time step different from the TH one.
- Introduce a control logic that calculate the next NK time step size to keep the error of the flux solution under a certain tolerance.
- Test the new coupling scheme on the High Temperature Test Reactor (HTTR) model for the LOFC transient in order to speed up the simulations and validate the code modifications.

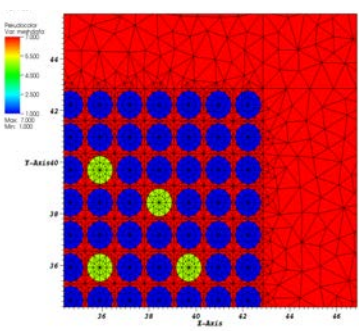


Code & Models

- **PHISICS** code modules overview
  - INSTANT: Transport/diffusion nodal solver, spherical harmonics based methodology, Second order formulation:
    - Unlimited number of energy group.
    - Spatial and angular discretization order up to 33
    - Cartesian 2/3D, Hex 2/3D, Unstructured Triangular, Wedges.
    - Adjoint calculations.
  - MRTAU: Bateman solver, CRAM, depletion evolution.
  - MIXER: Cross section manager, micro, macro or mixed, Unlimited number of tabulation parameters.
  - COUPLING: **RELAP5-3D©** coupled, for steady state and transient simulations.



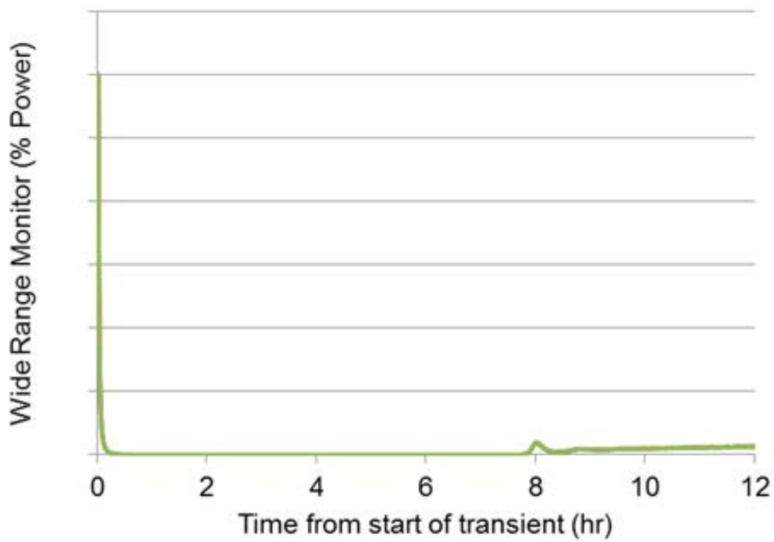


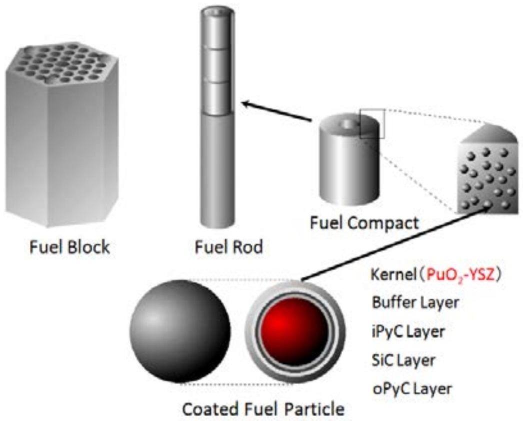


Code & Models

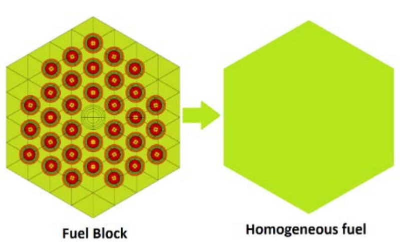
- The HTTR and LOFC transient
  - December 2010, JAEA performed a LOFC, with automatic reactor trip circuitry disabled.
  - When the forced flow stopped, the fuel temperature increased → negative reactivity → sub-critical within the first minute.
  - Critical again after 8h for the Xe^{135} decay

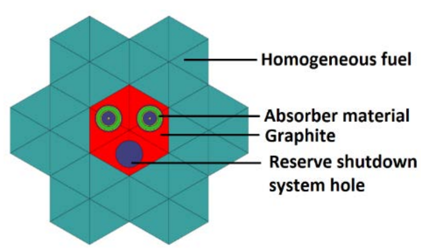
Reactor main parameters	
Power	30 MW
Coolant	Helium
Primary pressure	2.774 MPa
Average power density	2.5 W/cm³
Core diameter	2.9 m
Outlet coolant temperature	320°C
Inlet coolant temperature	180°C

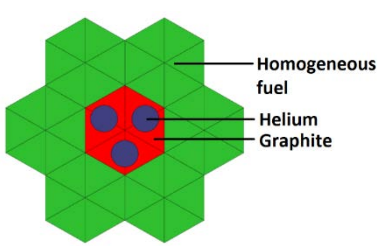




- HTTR 3D NK and TH model
  - TH model: One TH channel for each radial ring + conduction and radiation model.
  - NK model: 3D Hex assembly by assembly nodalization with 5 axial meshes for the active zone
  - XSec: mixed XSec generated using **DRAGON5**
    - Macro XSec for the FUEL.
    - Micro XSec with Xe^{135} and I^{135}.
    - Tabulated respect to Fuel, Moderator temperature, and Xe^{135} concentration

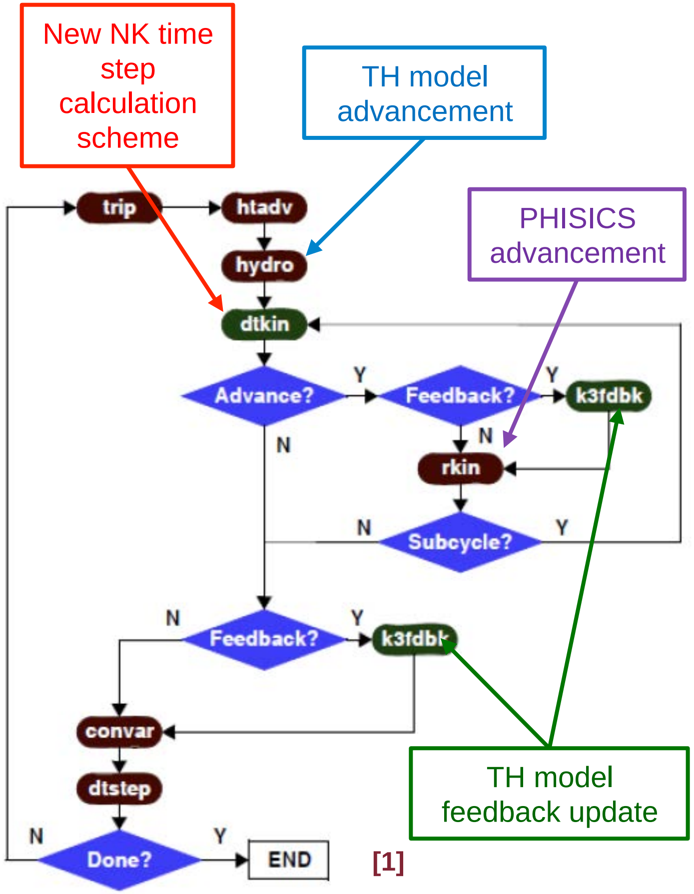






Decoupling scheme

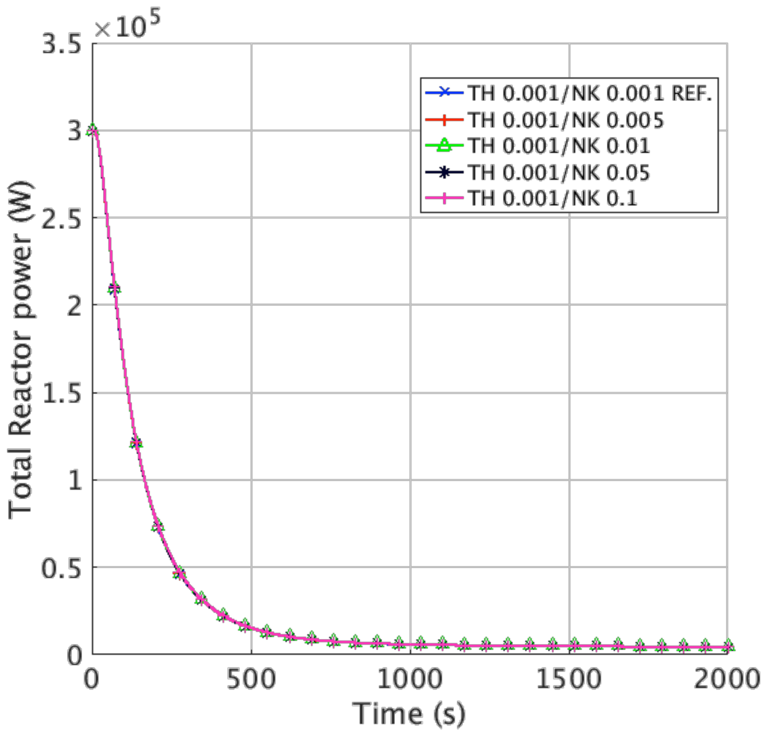
- Decoupling scheme
  - The **RELAP5-3D©** decoupling scheme developed for NESTLE has been used→ Minor modifications applied to the **PHISICS** code in order to use the new NK time step for MRTAU (depletion) and for the time evolution scheme.
  - To verify the functionality of the modifications with a simplified model, using the same **PHISICS** modules→ Reduced version of HTTR model→ one ring and one NK reflected assembly 15 axial nodes.

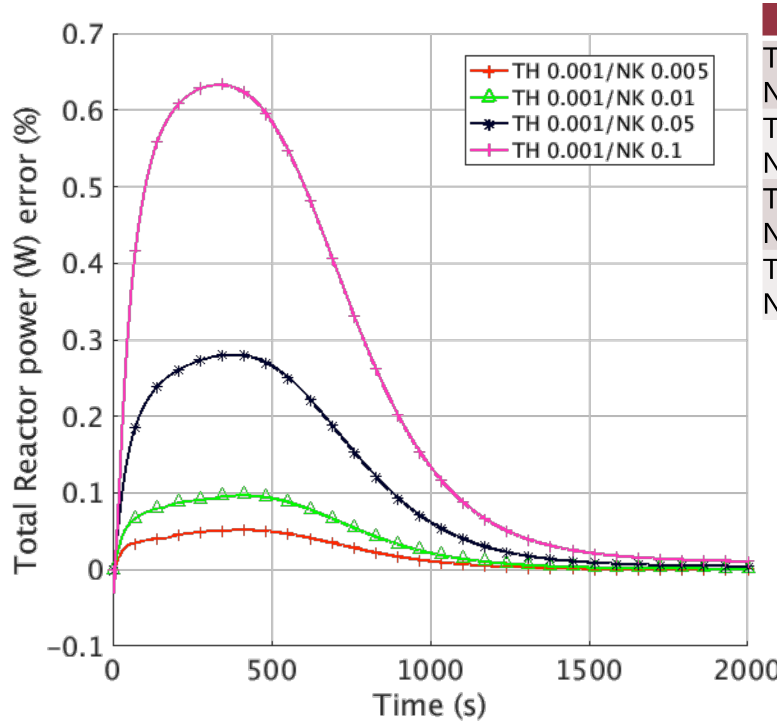


[1] D.Barber, "RELAP5-3D Model Improvement", International RELAP5 Users Group Meeting, Sun Valley, Idaho, 2012

Decoupling scheme

- Constant NK Time step results for time step decoupling scheme testing
  - Reference solution $\Delta t_{NK}=\Delta t_{TH}$=1e-3s for 2000 s transient (2E+6 iterations)
  - The Δt_{TH} has been kept to 1e-3s to ensure that the TH solution is fully converged and does not introduce error in the calculations.





Case	Speedup
TH 0.001 NK 0.005	3
TH 0.001 NK 0.01	5
TH 0.001 NK 0.05	8
TH 0.001 NK 0.1	14

WARNING: THERE IS NO CONTROL ON THE NK SOLUTION ERROR!!!

Adaptive time step

- Adaptive time step calculation scheme:

$$\frac{\partial \phi_r^g}{\partial t}\Big|_{t=t_n} = \frac{\phi_r^g(n) - \phi_r^g(n-1)}{\Delta t_n} + e_\phi^{(n)}$$

$$e_\phi^{(n)} = \frac{\Delta t_n}{2} \frac{\partial^2 \phi_r^g}{\partial t^2}\Big|_{t=t_n} + O(\Delta t_n^2)$$

$$e_\phi^{(n)} \Delta t_n \leq \tau$$

Predicted Time step

$$\Delta t_p \leq \sqrt{2\tau \left|\frac{\partial^2 \phi_r^g}{\partial t^2}\right|^{-1}}$$

Additional constrains

1) $0.001 \leq \Delta t_p \leq$ 2.0 s
2) Δt_p rational multiple of the Δt_{TH}

Methodology 1 (M1)

$$\frac{\partial^2 \phi_r^g}{\partial t^2}\Big|_{t=t_n} \approx \frac{\Delta t_{n-1}\phi_r^g(n) - (\Delta t_{n-1} + \Delta t_n)\phi_r^g(n-1) + \Delta t_n \phi_r^g(n-2)}{\Delta t_{n-1}\Delta t_n(\Delta t_{n-1} + \Delta t_n)}$$

Methodology 2 (M2) [2]

$$\frac{\partial^2 \phi_r^g}{\partial t^2}\Big|_{t=t_n} \approx \frac{\Delta t_{n-1}\phi_r^g(n) - (\Delta t_{n-1} + \Delta t_n)\phi_r^g(n-1) + \Delta t_n \phi_r^g(n-2)}{\Delta t_n \Delta t_n \Delta t_{n-1}}$$

[2] M. W. Hackemack, J. M. Pounders, "Implementation of an a priori time step estimator for the multigroup neutron diffusion equation in asynchronously coupled RELAP5-3D", PHYSOR 2014, The Westin Miyako, Kyoto, Japan, 2014

Adaptive time step

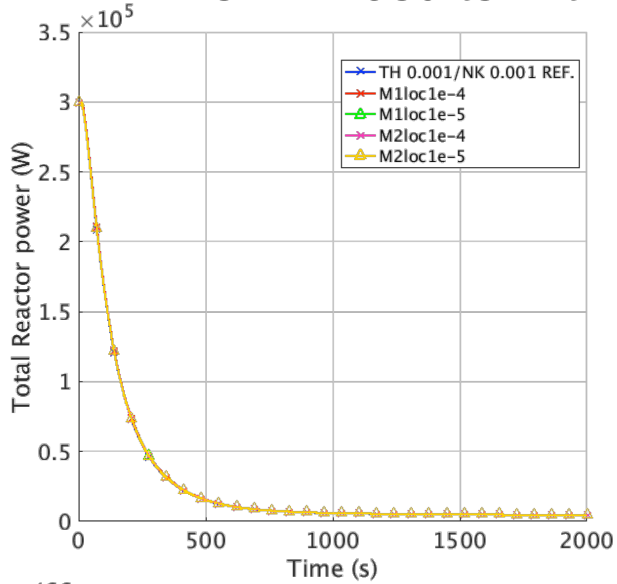
- M1 vs M2 results with local tolerance:

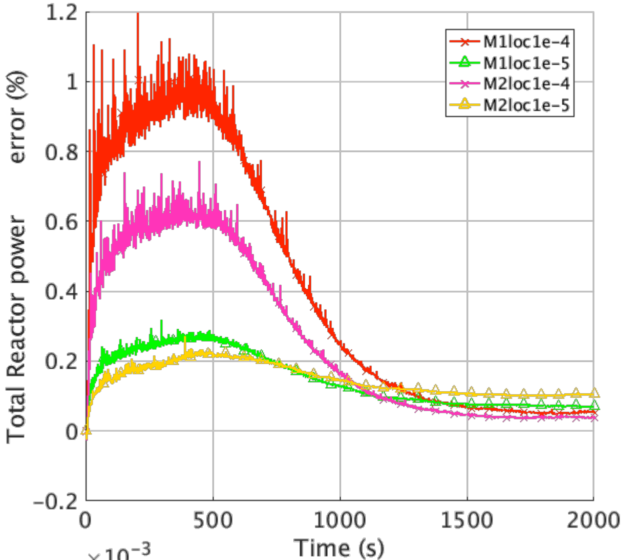
Case	Speedup
M1loc ε=1e-4	18
M1loc ε=1e-5	**7**
M2loc ε=1e-4	12
M2loc ε=1e-5	6

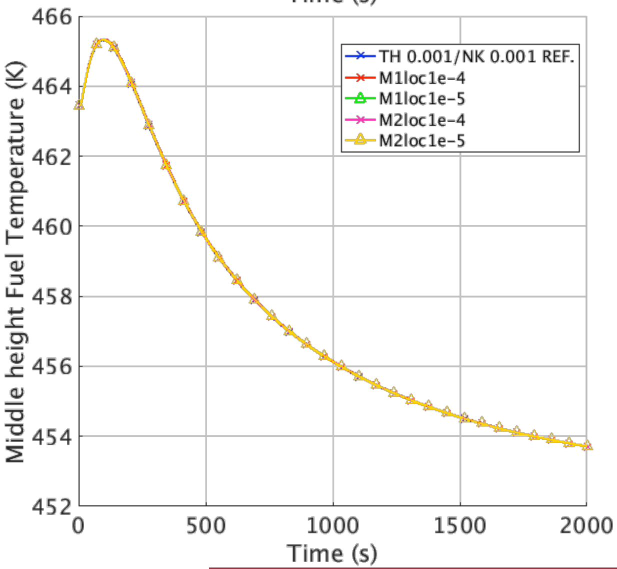
Local Tolerance

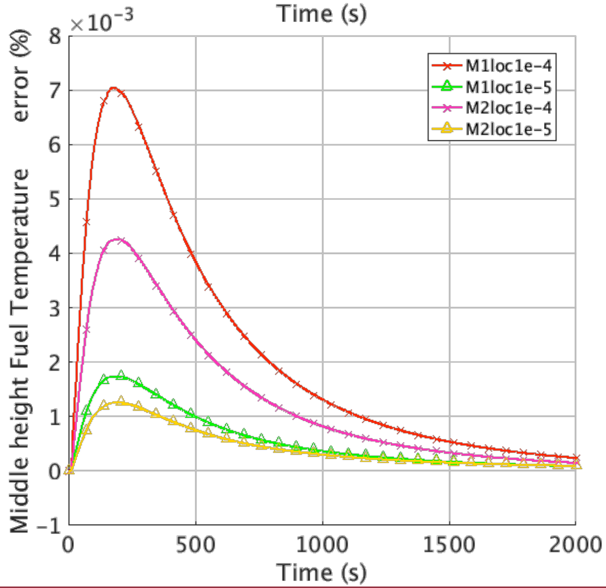
$$\Delta t_n = \min\left(\sqrt{2\tau \left| \frac{\partial^2 \phi_r^g}{\partial t^2} \right|^{-1}} \right)$$

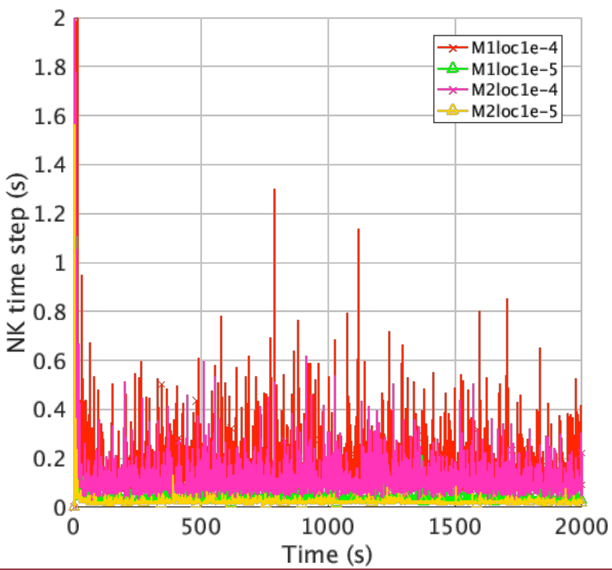
$$\tau = \varepsilon \phi_r^g$$





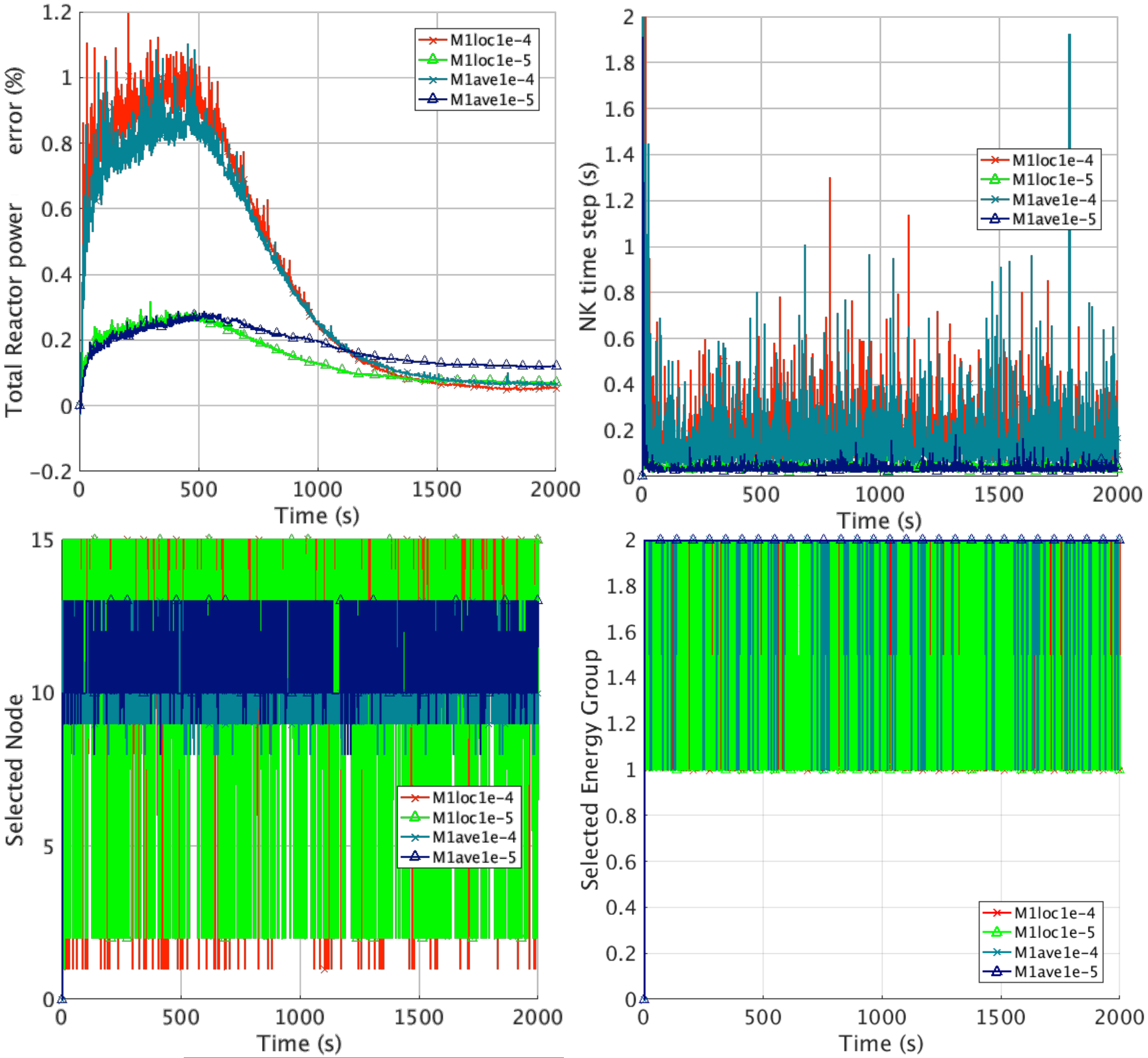






Adaptive time step

- Average tolerance vs local tolerance results



Case	Speedup
M1loc ε=1e-4	18
M1loc ε=1e-5	7
M1ave ε=1e-4	15
M1ave ε=1e-5	7

Average flux Tolerance

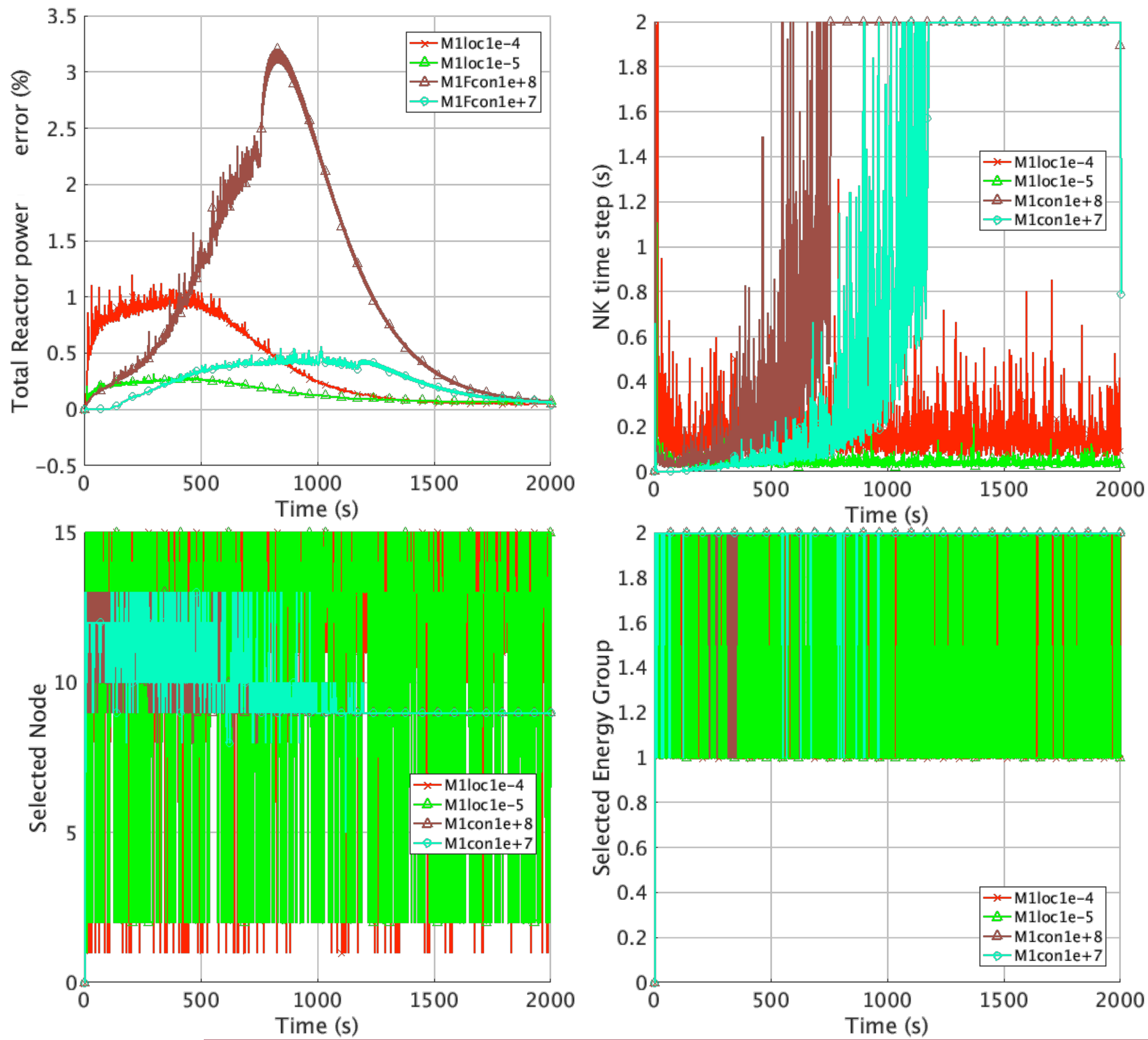
$$\Delta t_n = \min\left(\sqrt{2\tau \left| \frac{\partial^2 \phi_r^g}{\partial t^2} \right|^{-1}}\right)$$

$$\tau = \varepsilon \phi$$

N.B. the tolerance is proportional to average flux but the second derivative is still calculated in each node and energy group

Adaptive time step

- Constant tolerance vs local tolerance results



Case	Speedup
M1loc ε=1e-4	18
M1loc ε=1e-5	**7**
M1con ε=1e+8	33
M1con ε=1e+7	10

Constant Tolerance

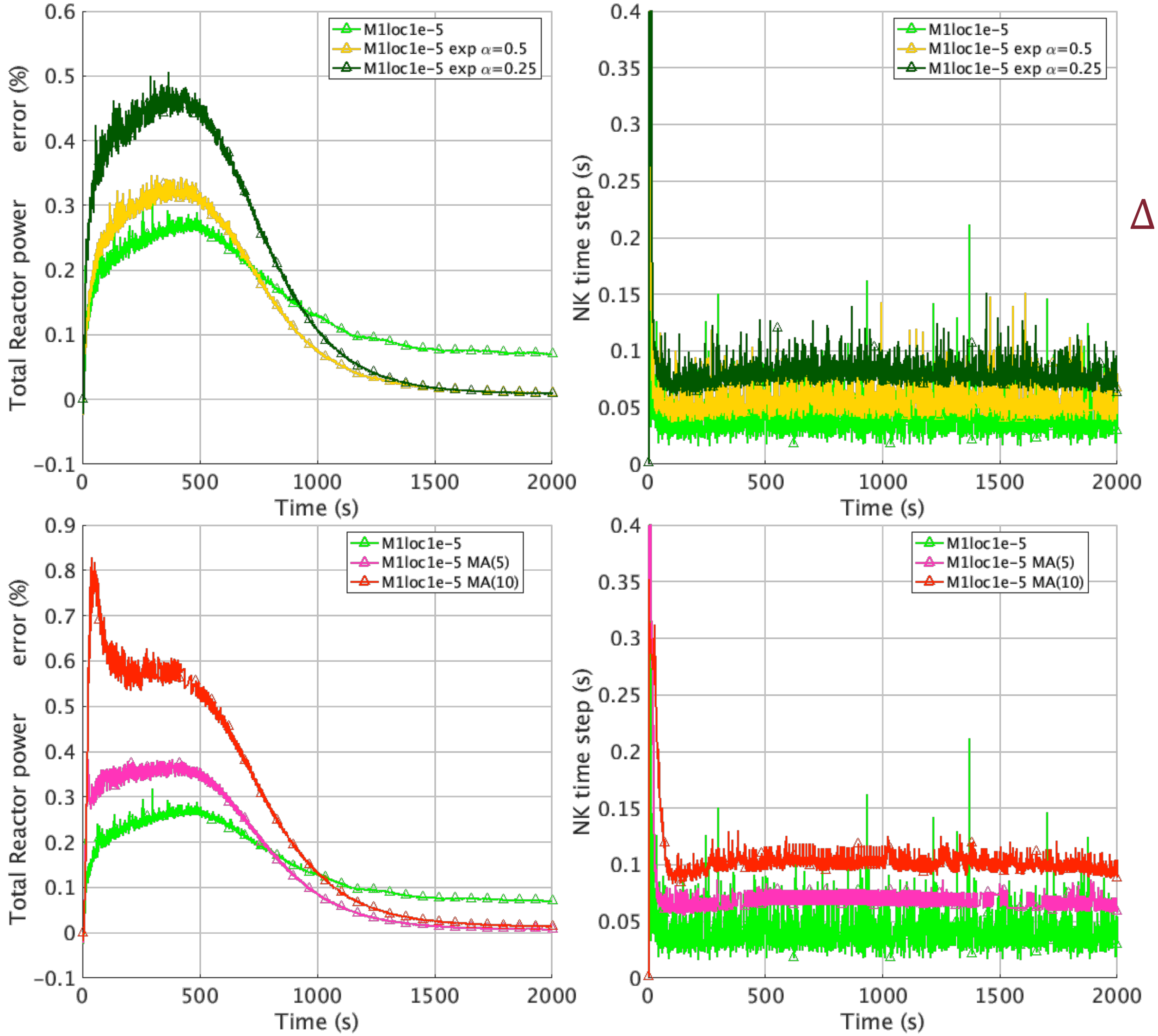
$$\Delta t_n = \min\left(\sqrt{2\tau}\left|\frac{\partial^2 \phi_r^g}{\partial t^2}\right|^{-1}\right)$$

$\tau = \varepsilon$ [n/cm2/s]

N.B. the tolerance is proportional to average flux but the second derivative is still calculated in each node and energy group.

Adaptive time step

- Moving average (MA) and Exponential smoothing on NK Δt prediction



Exponential smoothing

$$\Delta t_n = \Delta t_{n-1}(1-\alpha)+\alpha\Delta t_{p}$$

Moving average MA(N)

$$\Delta t_n = \sum_{i=1}^{N-1} \Delta t_{n-}$$

Case	Speedup
M1loc ε=1e-5	**7**
M1loc ε=1e-5 α=0.5	8
M1loc ε=1e-5 α=0.75	11
M1loc ε=1e-5 MA(5)	10
M1loc ε=1e-5 MA(10)	14

Conclusion & future steps

- The **RELAP5-3D©** decoupling scheme has been successfully modified and verified for the **PHISICS** code. All the **PHISICS** modules used in the HTTR model are now compatible with the new decoupling scheme.
- **Two** different Methodologies for the flux error estimation has been introduce. **Three** different kind of tolerance can be used to control the flux error trough the time step size. **Two** smoothing techniques are available to reduce the time step noise.
- More than **100** run with a simplified version of the HTTR model has been performed to test the best combination of methodology, tolerance definition, and smoothing.
- Future steps:
  - Test the modifications on the full HTTR model and the full LOFC (>40000 s)
  - Implement a third methodology for the time step prediction based on an more stable implicit scheme developed in [3].
  - Test the possibility of using some "hybrid methodology" using different methodology simultaneously. Introduce the flux extrapolation option.
  - Implement the quasi-static approach for very long transients (>1d).

[3] C.Rabiti, "Modelling of Fast Neutron Transients in an Accelerator Driven System", IKE, 2007

International REALP5 Users Group Meeting And Training Seminars

New RELAP5-3D Lead and LBE thermophysical properties implementation for safety analysis of Gen IV reactors

Idaho Falls, ID October 7, 2016

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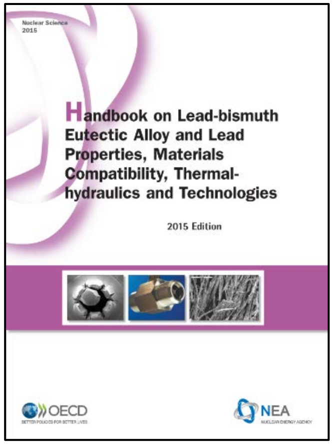
- The objective
- Thermophysical property comparison
- The soft sphere model
- Practical cases calculation and comparison
- Conclusions

The Objective

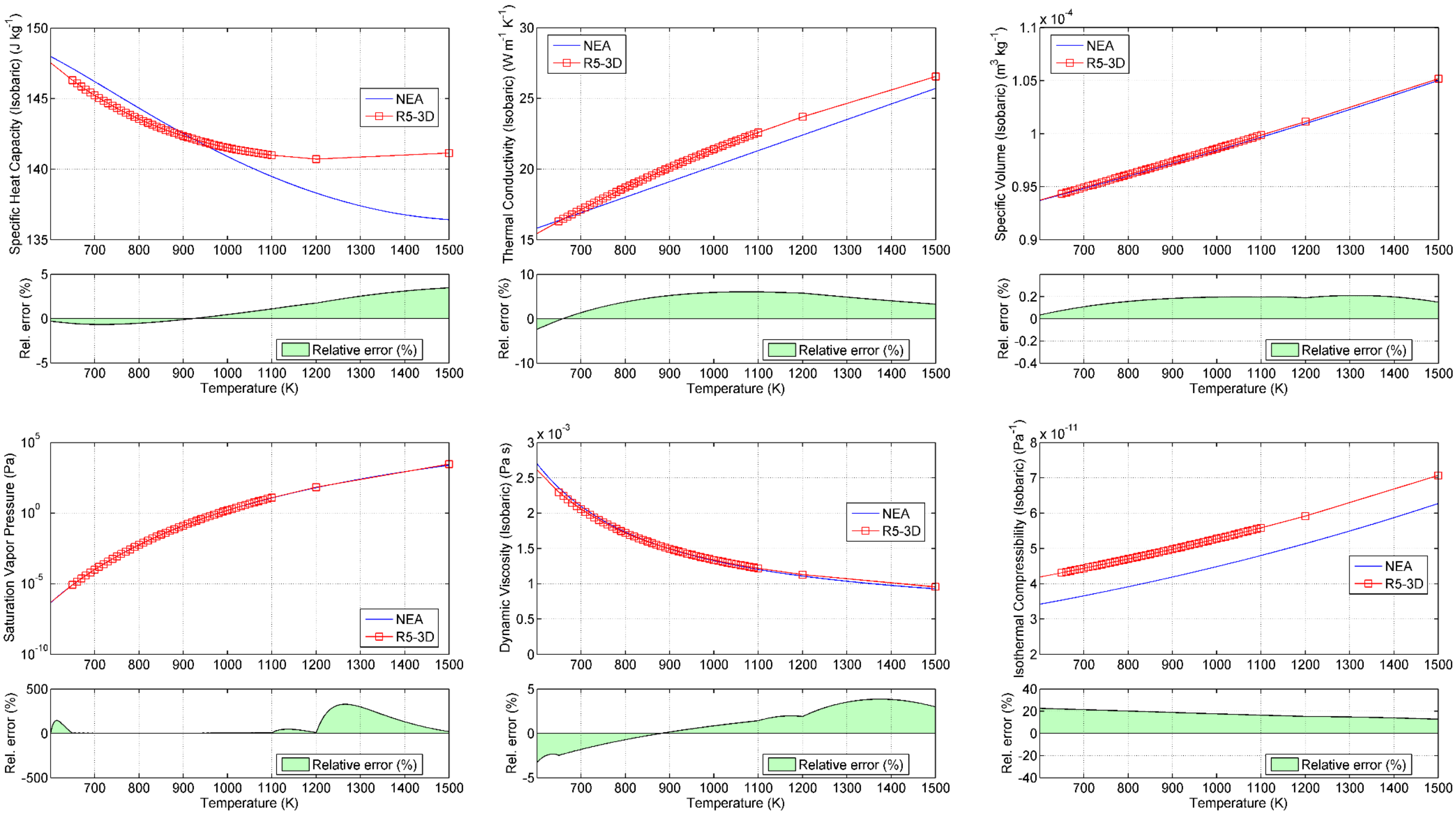
- Compare the RELAP5-3D© Lead and LBE thermophysical properties with the new one proposed in the 2015 NEA handbook.



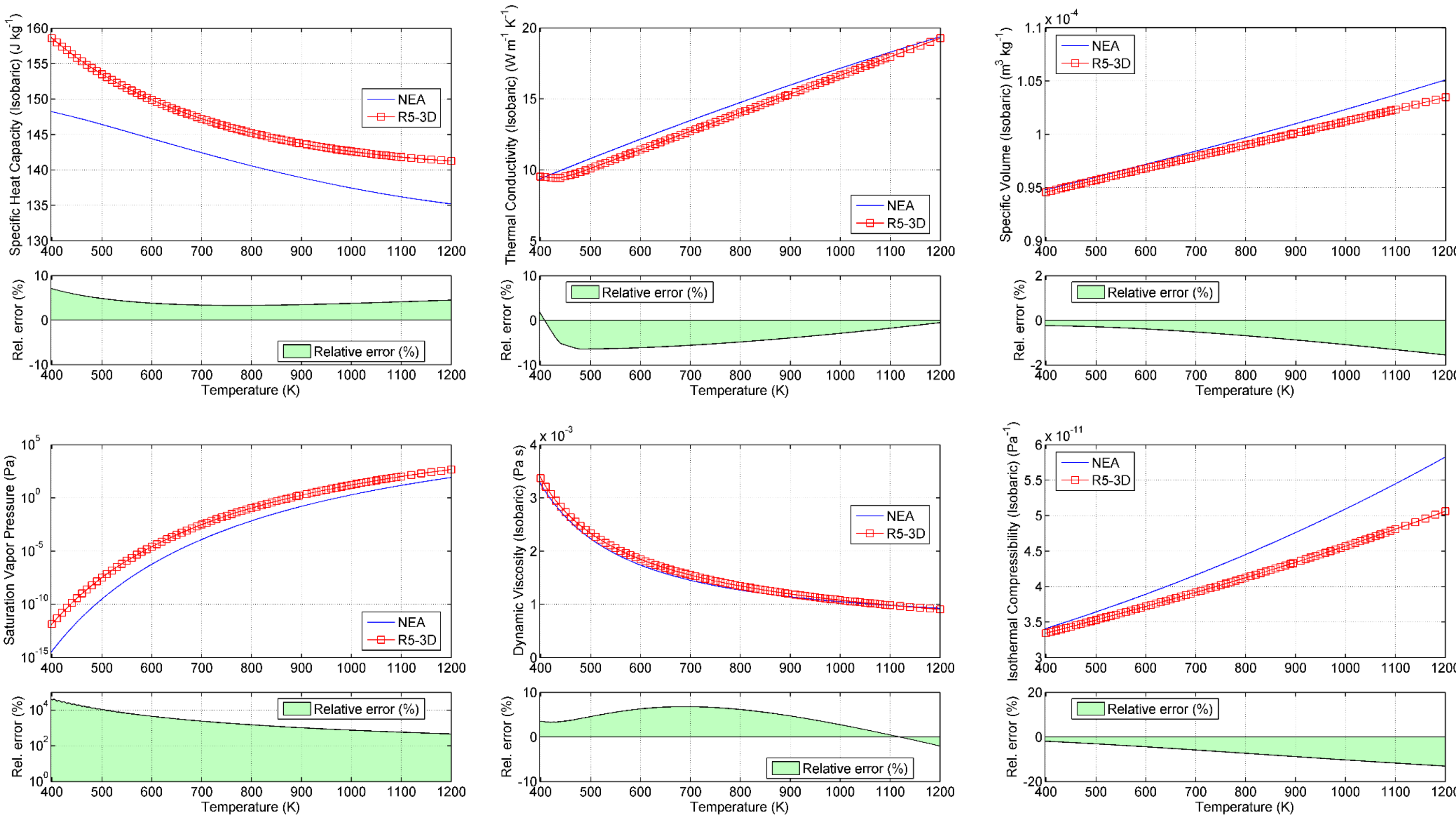
- Generate new thermophysical property files for LBE and Lead using a set of equation of state specific for the liquid metals fitted on the new NEA properties.
- Test and compare the effect of the new properties on the main parameters of a simple RELAP5-3D© model.

Thermophysical Property comparison

- Lead thermophysical properties R5-3D vs NEA 2015:



- LBE thermophysical properties R5-3D vs NEA 2015:



The soft sphere model

- Soft sphere model parameter optimization

Parameter to be optimized

$(n, m, Q, \sigma, \varepsilon, T)$

Error function definition

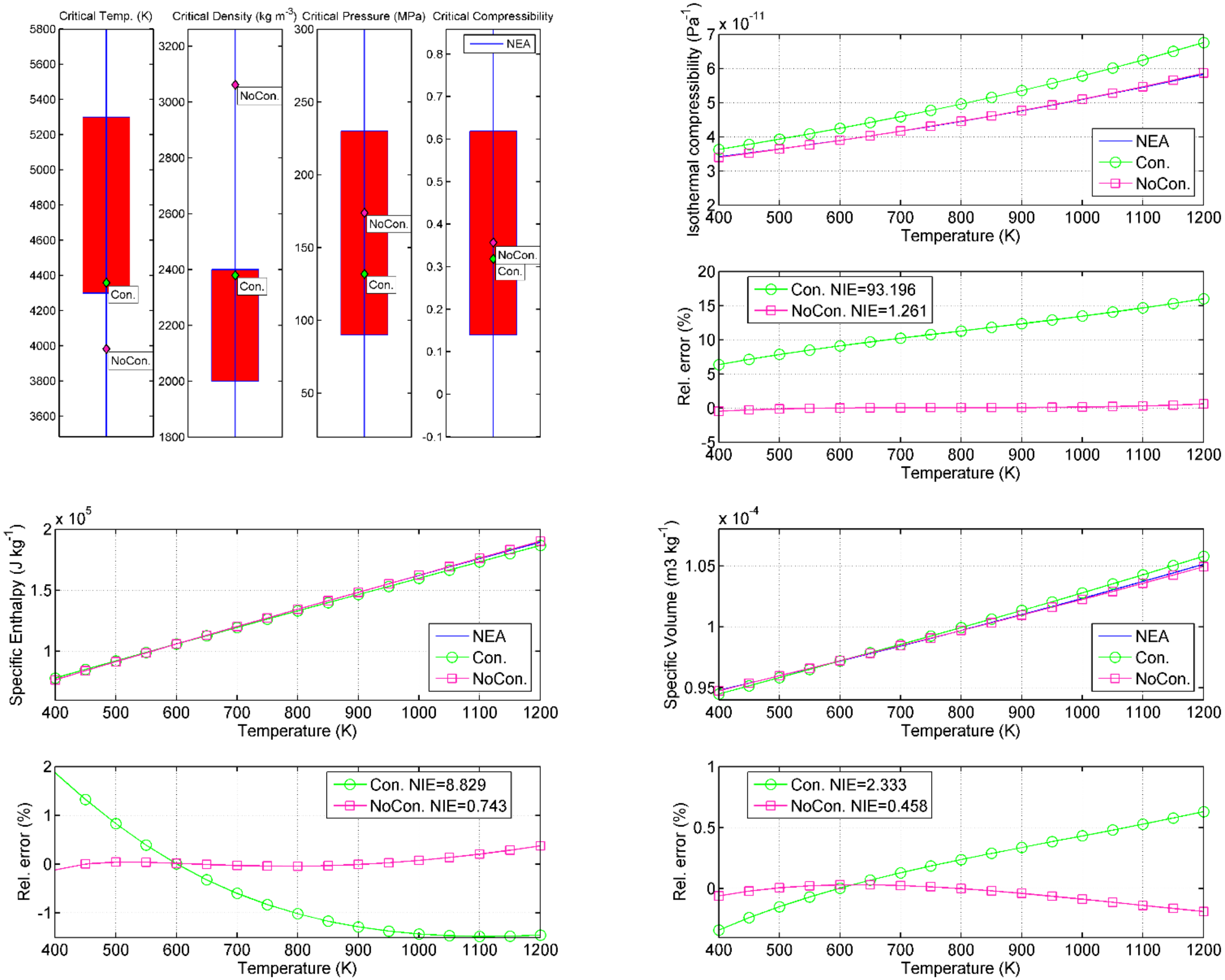
MEASURED DATA

- Specific volume (i=1)
- Specific enthalpy (i=2)
- Isothermal compressibility (i=3)

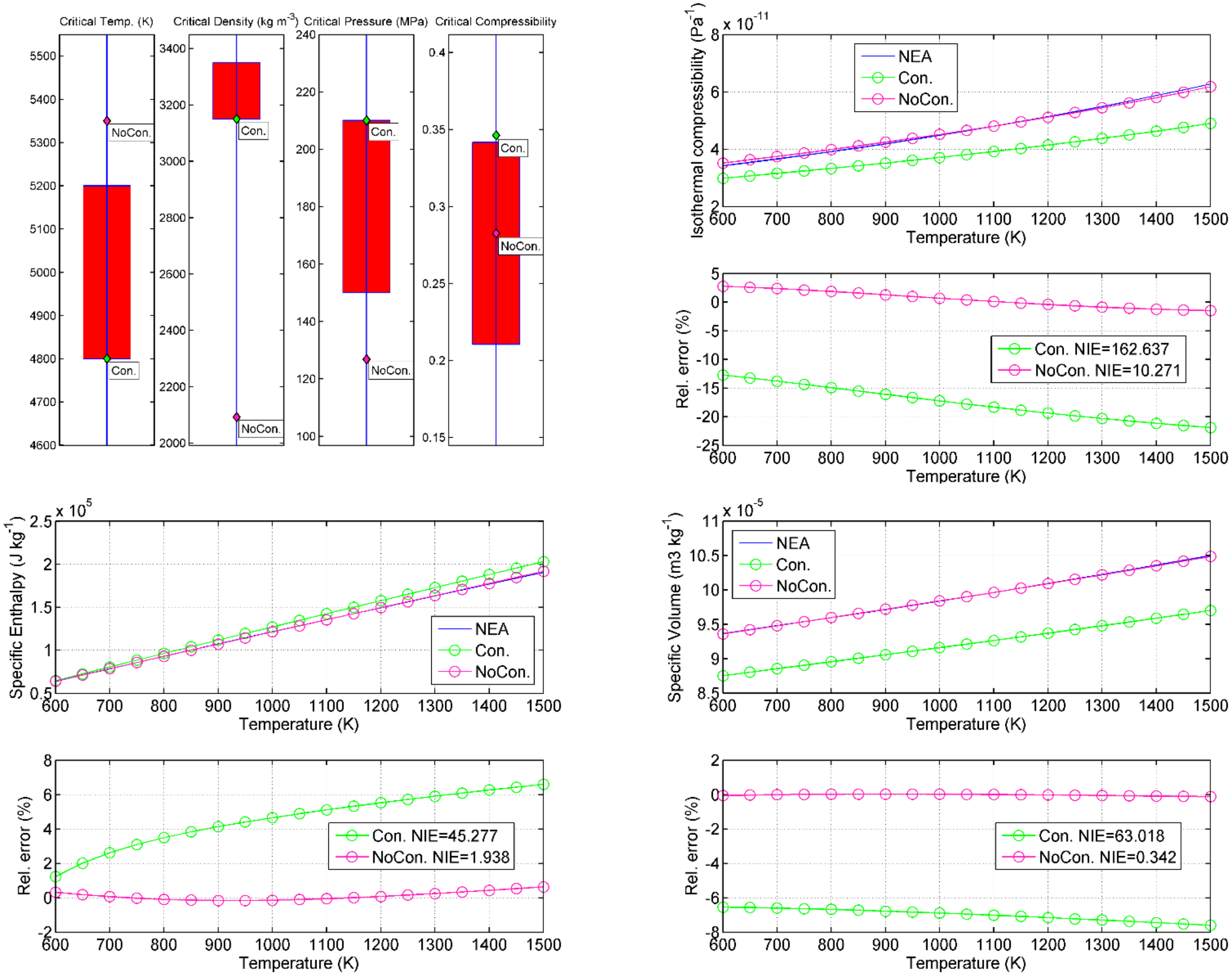
N.B available only for atmospheric pressure

The soft sphere model

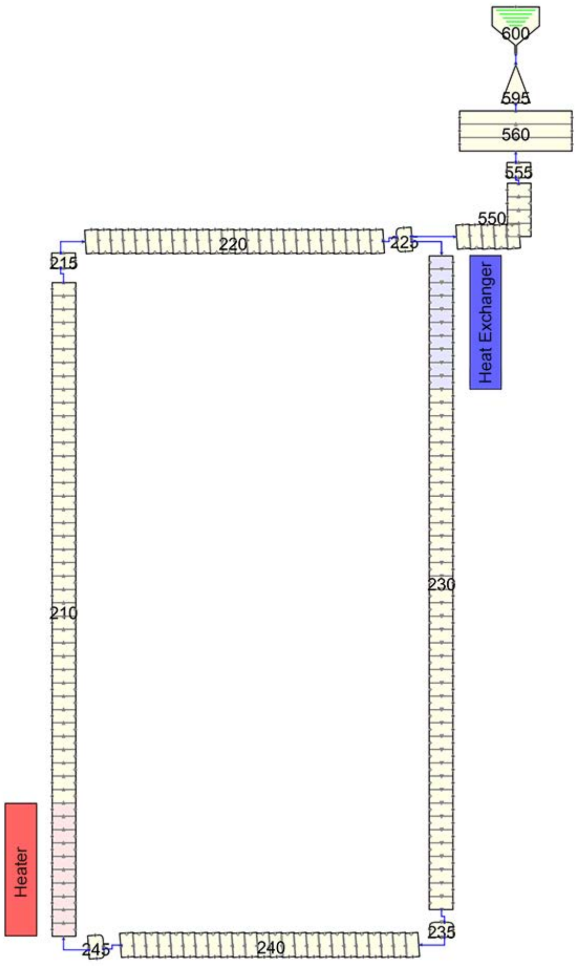
- Lead soft sphere model parameter optimization



- LBE soft sphere model parameter optimization



Simple natural circulation RELAP5-3D© model

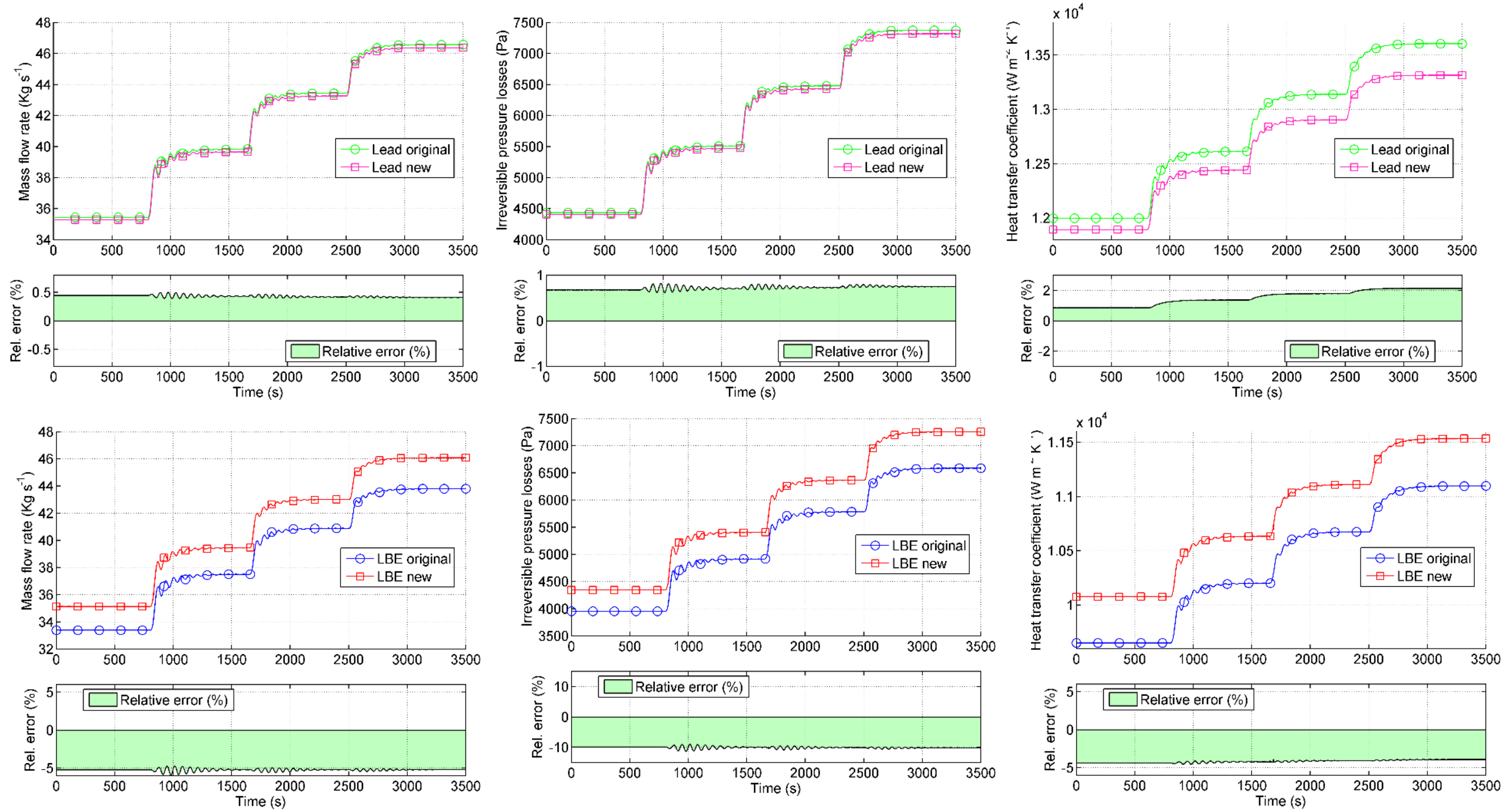


Parameter	Unit	Value
Flow area	m^2	$9.348 \cdot 10^{-3}$
Absolute roughness	m	10^{-5}
Heater steady state Power	kW	200.0
Heated section length	m	2.0
Heat sink wall temperature	K	610.0
Heat exchanger section length	m	2.0
Heat exchanger area	m^2	0.686
Heat exchanger wall thickness	m	$2.5 \cdot 10^{-3}$
Gas plenum pressure	Pa	$2.0 \cdot 10^5$
Vertical pipes length	m	10.0
Horizontal pipes length (4° vertical angle)	m	5.0
Expansion tank volume	m^3	0.36
Expansion tank height	m	0.6
Expansion tank level	m	0.3

- Lead and LBE Natural circulation loop main parameter comparison.

Lead

LBE



Conclusion & future steps

- Full comparison between the original R5-3D thermophysical properties and the NEA recommended ones has been reported for two heavy liquid metals, LBE and Lead
- A simple NC system has been used to compare the effect on the TH model main parameters.
- Lead properties show a limited discrepancy.
- LBE properties show a significant discrepancy, therefore further investigations and validation using experimental data should be performed.
- The future activities will be devoted to find an optimal pressure and temperature grid to minimize the numerical issues during the calculations and to the validation of the new thermophysical properties using experimental data.

Thank you for your attention !!!