Objectives

- Pyrolysis modelling capability for new flame retardants
- Quantification of the ageing effect for electrical cables
- Predicting the fire resistance of a barrier element
- Development and maintenance of fire modelling tools
- Participation in OECD PRISME project
Pyrolysis modelling of flame retardants

**Molecular Dynamics (MD):** A technique for computing the movement of atoms or molecules using classical equations of motion.

**Classical:** $F = ma$

- Give atoms initial positions $r^{(t=0)}$, choose short $\Delta t$
- Get forces $\mathbf{F} = -\nabla V(r^{(i)})$ and $a = \mathbf{F}/m$
- Move atoms: $r^{(i+1)} = r^{(i)} + v^{(i)} \Delta t + \frac{1}{2} a \Delta t^2 + \ldots$
- Move time forward: $t = t + \Delta t$
- Repeat as long as you need
Pyrolysis modelling of flame retardants

Reactive Molecular Dynamics (RMD): a version of the MD technique which allows chemical bonds to form and break

RMD can be used to predict pyrolysis chemistry
Pyrolysis modelling of flame retardants

Model system: PE + ATH (42 wt-%)
Pyrolysis modelling of flame retardants

Result: in fire temperatures, most of PE and ATH decompose independent of each other

A small chemical interaction between PE and ATH where hydroxyl radicals from ATH abstract hydrogen from PE
Pyrolysis modelling of flame retardants

Kinetic parameters for decomposition reactions can be obtained from RMD data using isoconvensional methods.

\[ k = A e^{-E_a/RT} \]

Heating rate

Temperature

Conversion

\( \ln(A) + \ln(f(\alpha)) \)

\( 1/T \)
Pyrolysis modelling of flame retardants

Kinetic parameters can be given to the pyrolysis model of a continuum-scale fire simulation (FDS)
Development of fire modelling tools

FDS: methodology to simulate effects of airplane impact on a nuclear island

Fig. 12. Near-field liquid dispersion pattern in test SFP5 with an impact velocity of 100 m/s and 25 L of water. The time instances are 1, 2 and 5 ms after the impact.
Development of fire modelling tools

FDS: methodology to simulate effects of airplane impact on a nuclear island
Development of fire modelling tools

FDS: pool fire HRR prediction in underventilated compartments

![Diagram of a fire model with labeled components and graphs showing fire rate over time for two different scenarios: PRS_SLD1, RR = 4.7 l/h and PRS_SLD6, RR = 4.7 l/h. The graphs compare experimental and simulated fire rates over time.]
Development of fire modelling tools

PyroPython: Python-based parameter identification tool

Pyrolysis of solids

Picture borrowed from: An extended pyrolysis model for cables in the context of PRISME2 fire tests
Spille, J. in PRISME2 final seminar

25.3.2019 VTT – beyond the obvious
Development of fire modelling tools

PyroPython is a successor for Pyroplot tool developed in earlier SAFIR projects

Programmed in Python, giving access to a rich open source ecosystem of scientific computing

Does not rely on Genetic Algorithm for parameter optimization; PyroPython can use any Python optimization toolbox (currently SciPy and Scikit-Optimize)

Easier to use than Pyroplot

Software online: [https://github.com/PyroId/PyroPython](https://github.com/PyroId/PyroPython)

Documentation online: [https://pyroid.github.io/](https://pyroid.github.io/)