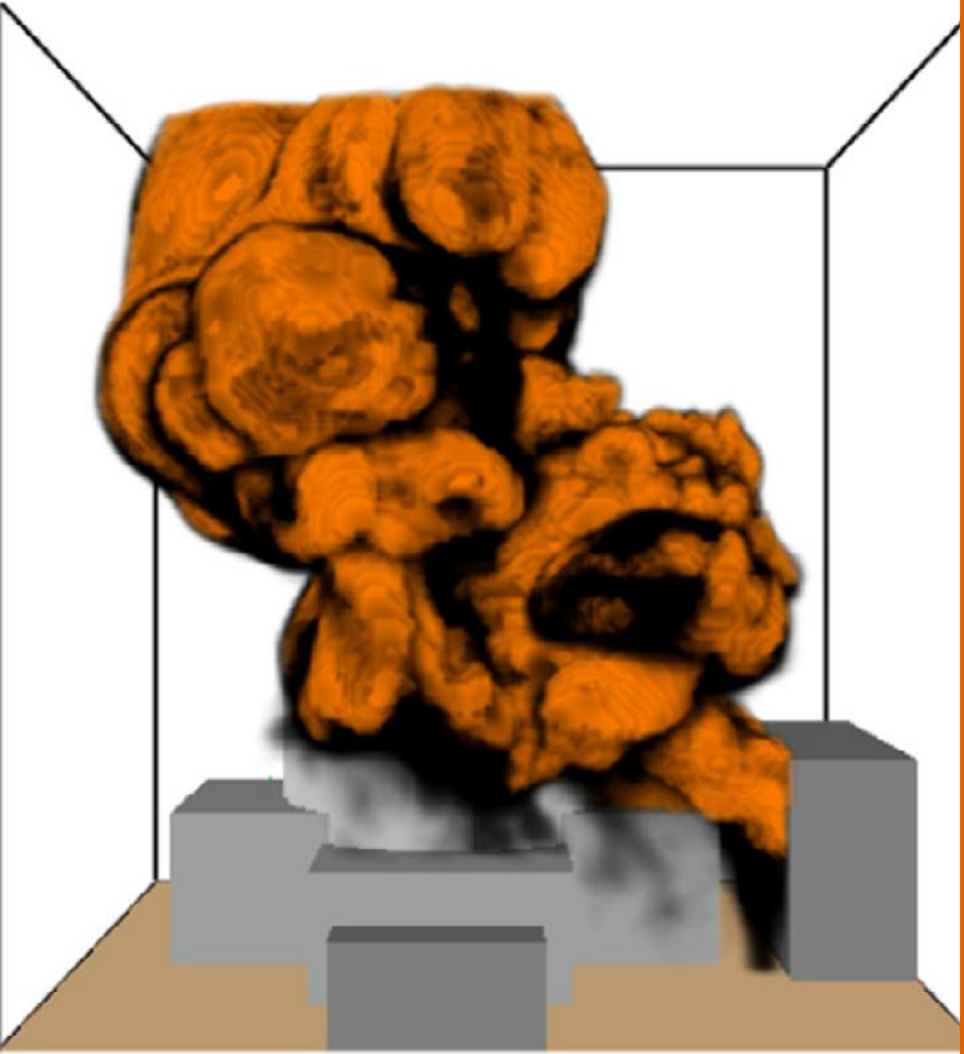


FIRED

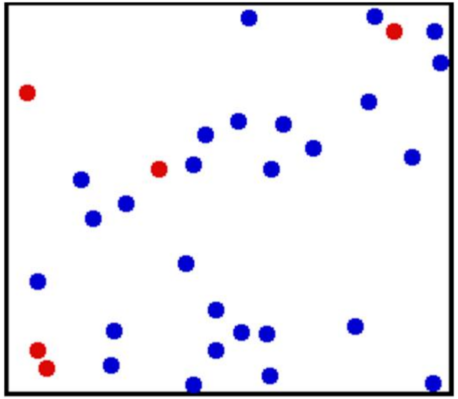
Jukka Vaari

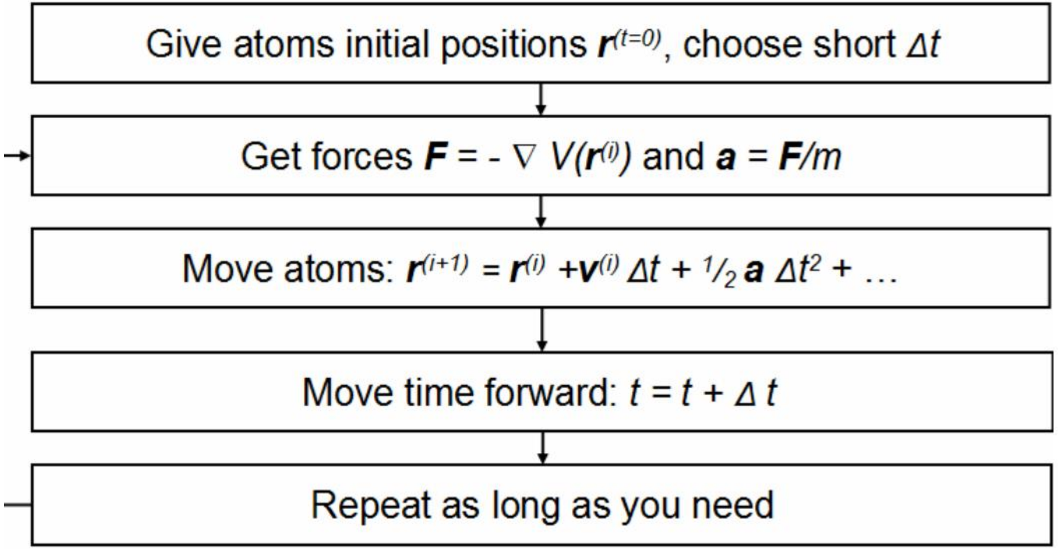
Objectives

- 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

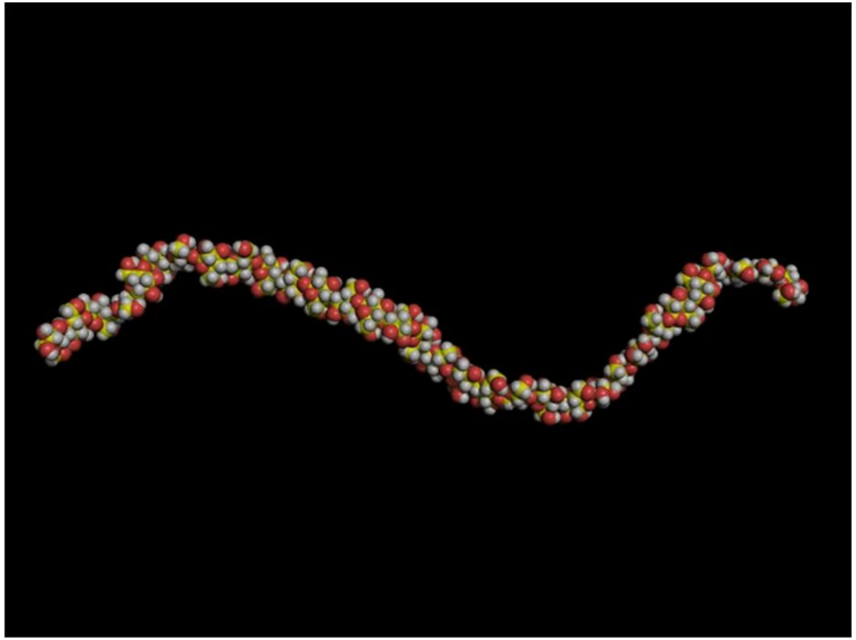
- Molecular Dynamics (MD): a technique for computing the movement of atoms or molecules using classical equations of motion
- Classical: F=ma





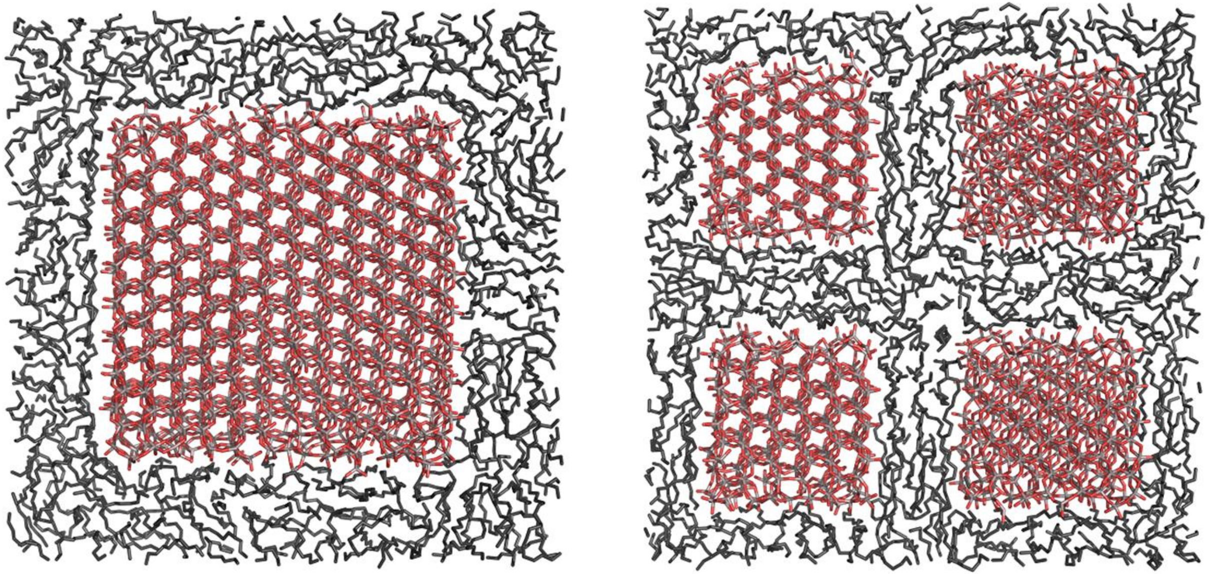
Pyrolysis modelling of flame retardants

- 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



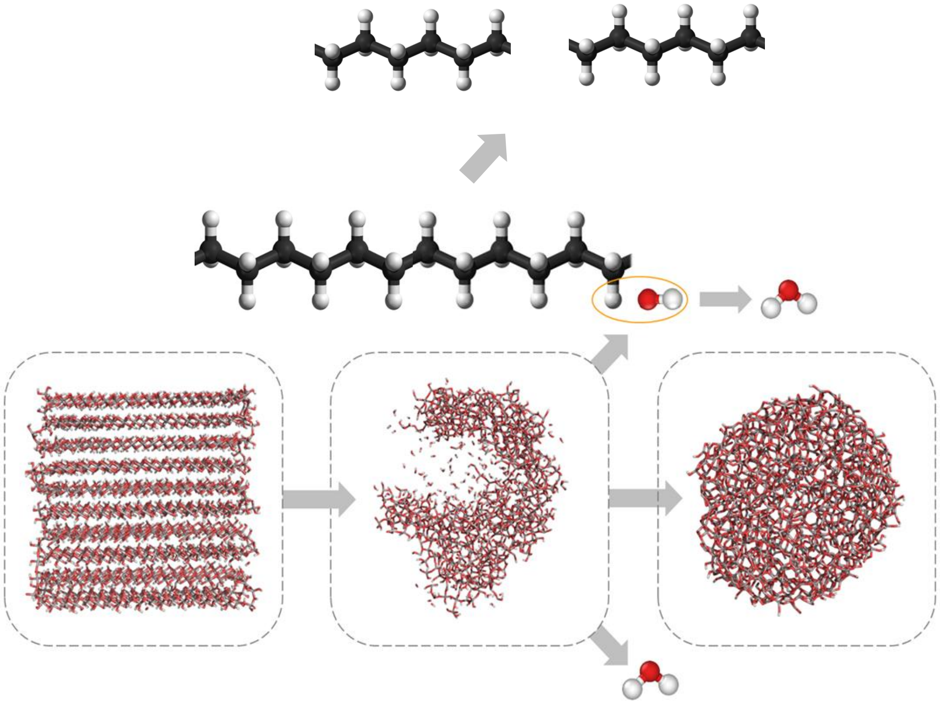
Pyrolysis modelling of flame retardants

- Model system: PE + ATH (42 wt-%)



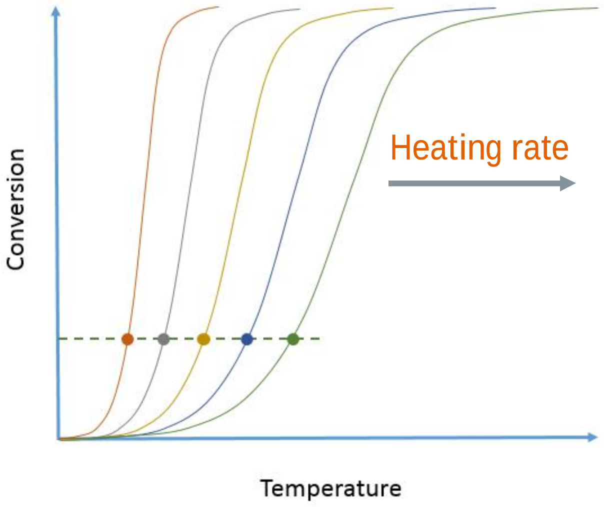
Pyrolysis modelling of flame retardants

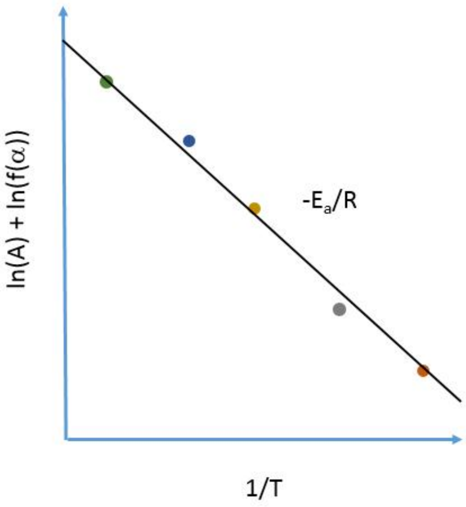
- Result: in fire temperatures, most of PE and ATH decompose independent of each other
- A small chemical interaction between PE and ATH where hydroxyl radicals from ATH abstract hydrogen from PE



Pyrolysis modelling of flame retardants

- Kinetic parameters for decomposition reactions can be obtained from RMD data using isoconversional methods

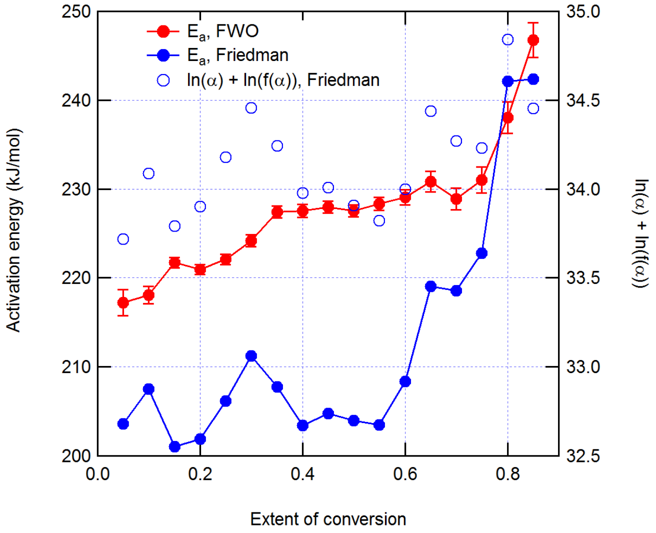


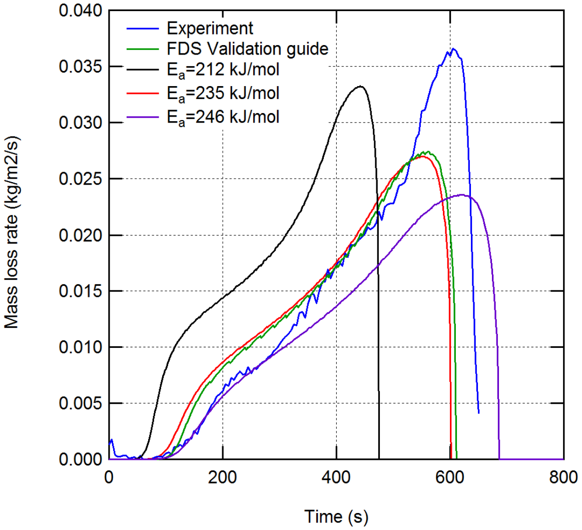


$$k = Ae^{-E_a/RT}$$

Pyrolysis modelling of flame retardants

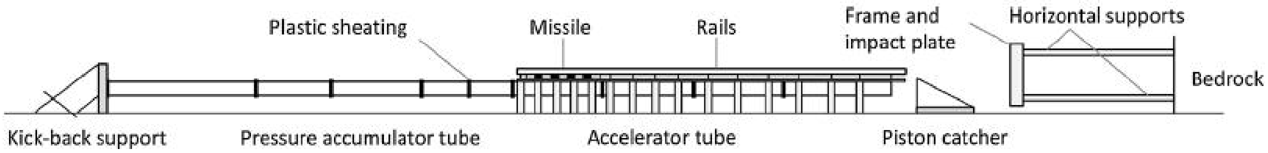
- Kinetic parameters can be given to the pyrolysis model of a continuum-scale fire simulation (FDS)



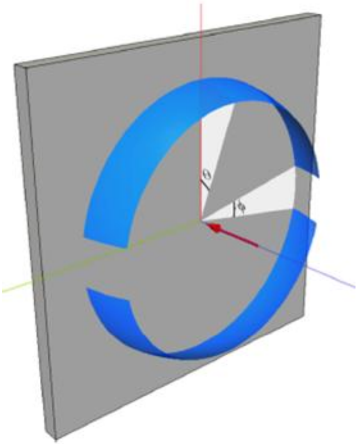


Development of fire modelling tools

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



S. Hostikka et al. / Nuclear Engineering and Design 295 (2015) 388–402



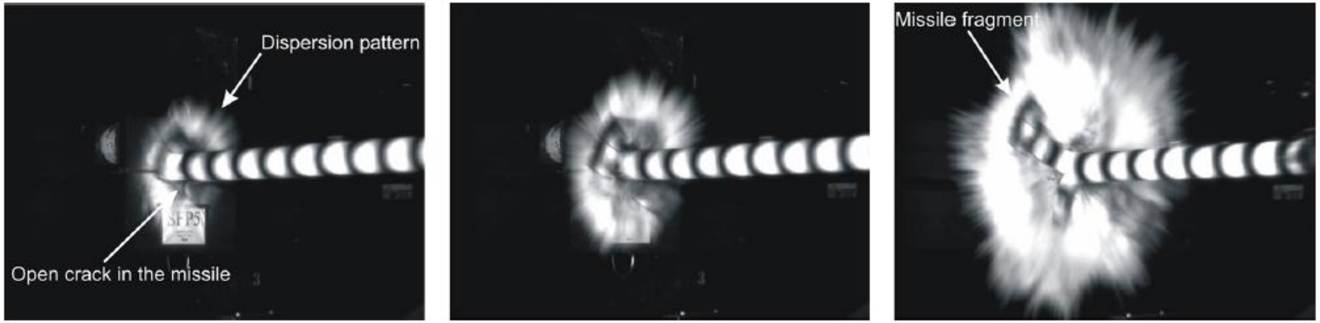
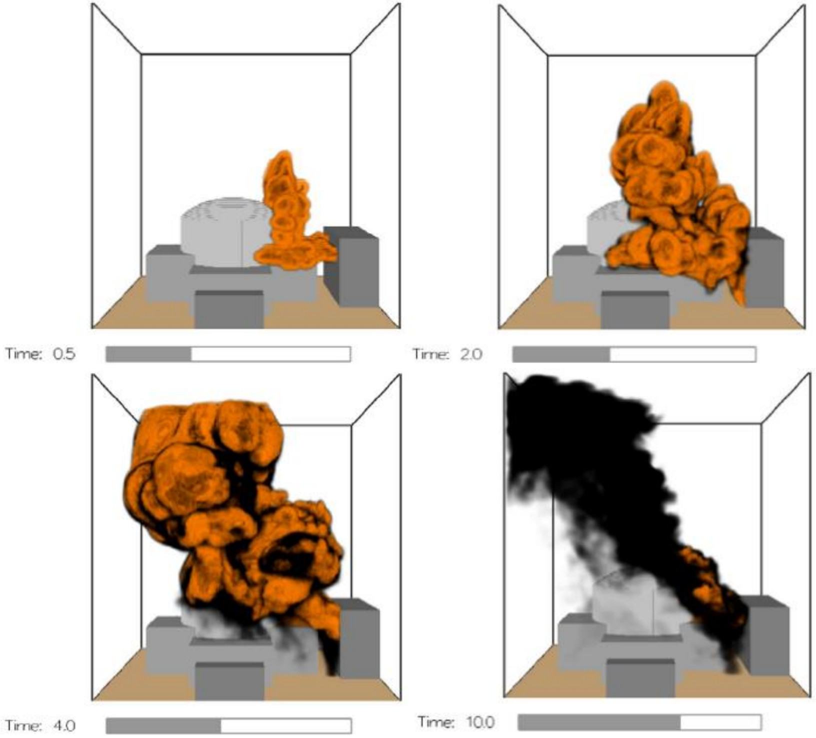


Fig. 12. Near-field liquid dispersion pattern in test SFP5 with an impact velocity of 100 m/s and 25 L of water. The time instances are 1, 2 and 5 ms after the impact.

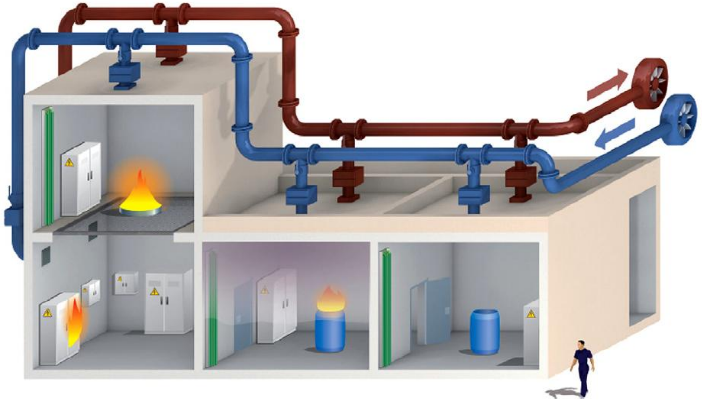
Development of fire modelling tools

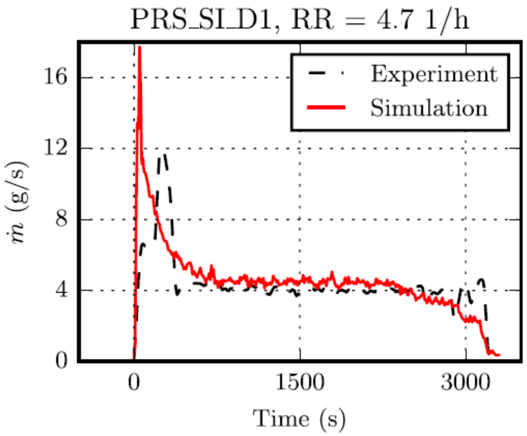
- FDS: methdology to simulate effects of airplane impact on a nuclear island

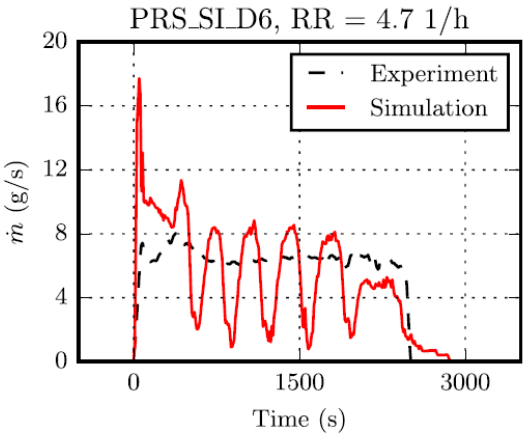


Development of fire modelling tools

- FDS: pool fire HRR prediction in underventilated compartments

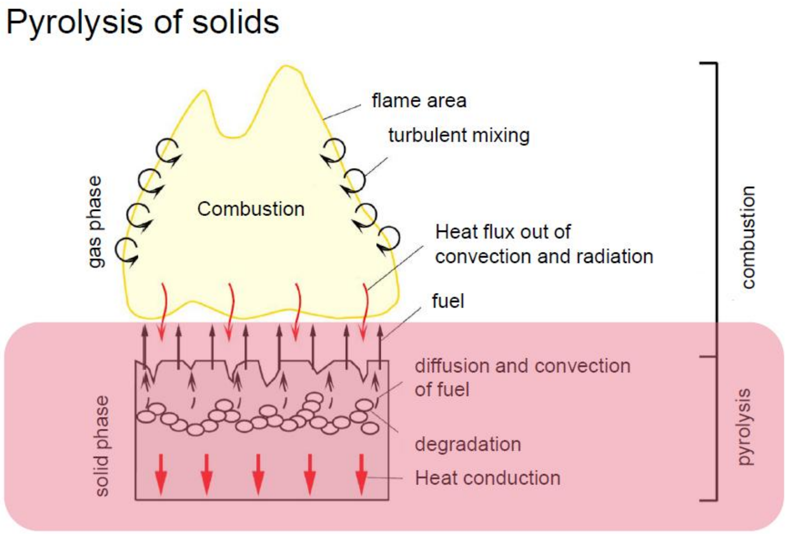


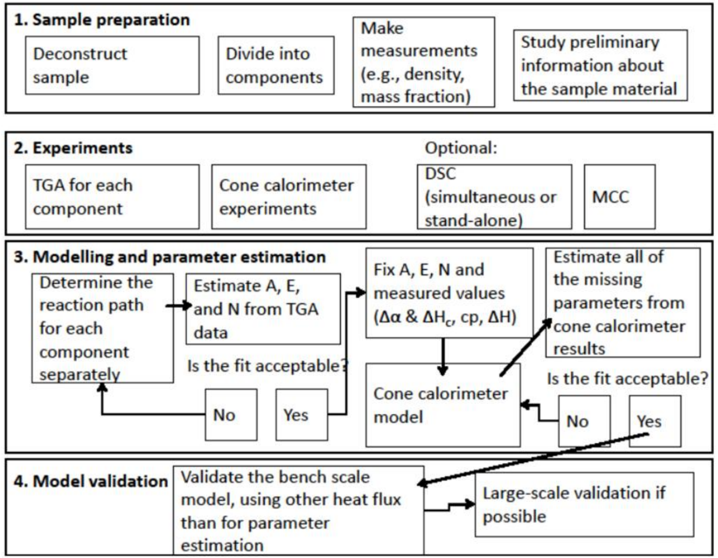




Development of fire modelling tools

- PyroPython: Python-based parameter identification tool





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

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
- Documentation online: https://pyroid.github.io/