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Simulation-based Assessment of Exposures with hazardous Substances
– Synergistic Application of Fire Engineering Models –

A.1 Risk assessment of hazardous substances

- Opportunities for risk assessment corresponding to GefStoffV (german regulation act):
  - Measurement and analogous review → comparable conditions necessary
  - Calculation → possibility of to predict concentrations
- Existing and used calculation models in occupational health and safety:
  - e.g. simple orientating estimations, emission-calculations, calculations of concentration in air; simplifying concepts
  - evident weakness in estimation of local concentration in air, e.g. assumption of localy-homogenous concentrations (admissibility to reality?)
  - uncertain application scopes, usually no validation or widescale restricted application scope

→ *Applicability to get „real“ calculation results?*

A.2 Fire Engineering: Smoke Management Simulation

- e.g. focussed on calculations to design the local- and time-depended smoke management
- Concept: fragmentation in calculation fields (typicaly 0,001-0,008m^3), time-depended solution of thermodynamic and dispersion parameters for each field (i.a. Navier-Stokes-Equations)
- Smoke: considerated as mixture of different (hazardous) substances, oppurtunity to solve dispersion equations without defined fire scenario and with detailing substanceous emission
  → Point of intersection with occupational safety studies as potential synergy
- benefit: local- and time-dependence, several validation studies for fire scenarios (heat release, increasing temperatures, bouyancy flows etc.)
  → *Focus of research: Possibility to applicate in occupational health and safety studies?*

A.3 Calculation Model: gaseous dispersion in air

- formal applicability of calculation systematic for occupational and fire safety studies
- common parameters: geometry, thermodynamic conditions, ventilation s.o.
- parameters for studies of smoke-dispersion:
  fire scenario with heat release (thermal force on dispersion etc.), emitted components and mass fractions in smoke (calculation of total mass flow)
- parameters for substanceous dispersion without fire:
  Substance with its properties, area of emission, emitted mass flow over area
  → without heat release: different parameters essential for dispersion (e.g. ventilation flows)
  → reasonable estimation of emission? assessment of calculated concentration in air?
  → *Supplementations to an integrated assessment concept, transferability?*

B.1 Integrated assessment concept

- Modular design (structural plan):
  - Determination of information: adjusted „working system“ to capture all needed parameters (to ensure completeness)
  - Capture of emission: approbriate choice from model pool (calculations, analogous assumptions by similarly cases, unnecessary in case of known emission parameters) and situation-dependend application
    Basis: determination of information in „working system“
  - Capture of dispersion: Application of fire engineering model „Fire Dynamics Simulator“ (FDS) [NIST, USA],
    Basis: determination of information in „working system“, area-weighted mass flow of emission as result of capture of emission (interface with conversion factor, if needed)

    - Assessment of exposures: identification of risks based on worker-to-concentration-coincidence
      Basis: determination of information in „working system", time- and local-dependend concentration in air as result of capture of dispersion (interface with conversion factor, if needed)
- Conceptual definition: structural procedure and internal interfaces
  → *Object of investigation*

B.2 Computational results

  - calculation results for dispersion: Properties of utilisation
    quantitative progress of concentration in air (tabular), e.g. graph over time
    → relation to limit values, comparing ventilation designs as basis for selection etc.
  - qualitative visualisation
    → local flows, time-dependend concentrations in air, risk communication etc.

→*Topics of research:*

  - *Calculation of dispersion:*
    Accuracy, application scope, validity as precondition for transferability?
  - *Integrated assessment concept:*
    Functionality modular design, definition of interfaces and conversion factors, validity of „full-case-calculation" (emission and dispersion)?

→ *Validation studies as basis for practical application*

C.1 Validation studies

- Investigation of research topics
- Approach: Measurement of reference concentrations in definied conditions, relation to calculated concentrations (calculation with conditions as input parameters)
  - Research-project funded by DGUV: Emission of propane, evaporation of isopropyl alcohol, variable conditions, different measure points
  - Data usuage of IPA-ExposureLaboratory: various substances, increasing-/decreasing-progresses of concentrations with known conditions, definied measure point
- Results of relations:
  - Calculation of dispersion with fire engineering model: for dot-like gaseous emission no validity, *validity for areal emission / evaporation*
    → *Demonstration of methodical transfer of the fire engineering model*
  - Integrated assessment concept: *Functionality determination of information and interfaces*, evaporation models without validity under used reference conditions, influence on calculation of dispersion (under-estimated concentrations in air)
    → no validity whit application of evaporation models („full-case-calculations") under investigated conditions

→ *Definition of application scope to calculate gaseous dispersion resp. to apply integrated assessment concept in occupational health and safety studies*

C.2 Applicability and practical scope

- Basis: Results of research (correct interfaces, validity calculation of gaseous dispersion, no validity of emission-calculations) and identified preconditions
- Application scope i.a.:
  - Dispersion of gases, „normal-temperature"
  - waiver of calculated emission-mass-flows (other estimation necessary)
  - known substance and properties (or detailled estimation)
  - areal emission with known conditions (area, mass flow etc.)
  - known ventilation conditions (area, volume flow s.o.)
  - safety factors (e.g. ventilation rates and high emission-mass-flows)
  - Accuracy of calculation increases with precision of input parameters
- potential scopes in occupational health and safety studies i.a.:
  - situation-specific risk assessment (relation to limit values, defining precautionary systems) → high effort!
  - Defining practical tools and configuration guides for typical working situations (e.g. for branches)
  - forensic analysis and reconstroction of exposure situations for workers

→***Expert-Tool to estimate substance-specific risk as option for practical applications***