Validation of the Semi-empirical radiation model OSRAMO II for large pool fires

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1.0 Short overview of actual radiation models

- *Semi-empirical* models

  These models are widespread

- *Zone* models
  - 2 – 20 zones
  - Conservation equations for overall mass and energy
  - Relatively simple, short computational time

- *Field* models

  Time averaged Navier-Stokes-equations of fluid flow with sub-models
  - In general no combustion is involved
  - Mathematically complex
  - Significant run times on large computer systems

- *Integral* models

A compromise between semi-empirical models and field models

- Mathematically formulated in the same way as field models. They can contain sub-models of the turbulence structure, combustion and heat transfer processes.
- Demanding far less computer time than field models
- Up to the present there are no integral models which could be used for the prediction of large-scale pool fire hazard consequences

☐ *Co*mputational *F*luid *D*ynamics *(CFD)* field modeling approaches

- ○ DNS field model for pool flames with d ≤ 2 cm [*A. Schönbucher, Th. Koch, S. Staus, 1996*]
- ○ *Extended* DNS field model for pool flames with d ≤ 30 cm [*A. Schönbucher, S. Staus, 1999*]
- ○ Commercial ANSYS CFX-5.7.1 CFD software; ANSYS ICEM CFD 5.1 [A. Schönbucher, C. Kuhr (since 2000), I. Vela (since 2003)]

Steady state, semi-empirical simulation models for pool fires on land

1.1 *Point source* radiation model (PS):

J. Moorhouse (1982)

1.2 *Surface emitter* models

1.2.1 Solid flame radiation model (ZFS):

P.G. Seeger (1971)

1.2.2 Two zone radiation model (ZZ):

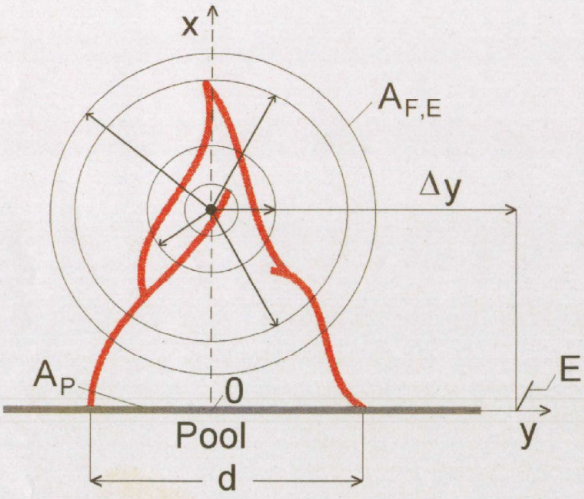
K.S. Mudan (1993)

1.2.3 *O*rganized *S*tructures *RA*diation *MO*del (OSRAMO II):

A. Schönbucher et al. (1985, 1991, 1999)

1.1 Point source radiation model (PS)

$$\overline{E}_{PS} = \frac{f_{rad}\,\dot{m}''_f A_P(-\Delta h_c)}{4a\pi\Delta y^2} \equiv \frac{f_{rad}\,\overline{\dot{Q}}_{ges}}{4a\pi\Delta y^2}$$



$\overline{E}_{PS}$ (Δy)	[W/m²]	thermal radiation flux resp. irradiance of the flame
f_{rad} (d,fuel)	[–]	fraction of the combustion energy radiated from the flame surface
$\dot{m}''_f$	[kg/(m²s)]	mass burning rate; $\dot{m}''_f = \rho_f v_a$ [v_a [m/s] : burning velocity resp. burning rate
a		empirical factor (a = 1)
Δh_c	[J/kg]	specific combustion enthalpy
A_P	[m²]	pool sectional area; $A_P = \pi d^2 / 4$
Δy	[m]	distance between the source and the receiver element of area; spherical surface: $A_{F,E} = 4\pi\Delta y^2$
$\overline{\dot{Q}}_{ges}$	[W]	total heat power resp. total heat release rate of the fire; $\dot{Q}_{ges} = \dot{q}''_f A_P = \dot{m}''_f(-\Delta h_c)A_P$
$\dot{q}''_f$	[W/m²]	total heat power per pool sectional area

Application:

- $\Delta y > 5d$
- for gas fires
- for pool/tank fires

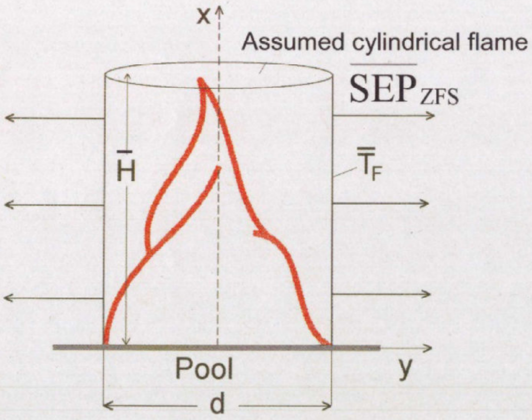
WHAZAN ($a \neq 1$):

$A_P = \pi d^2/4 + \pi dH$;
$a = c_1\,\dot{m}''^{0.61}_f + 1$;
$c_1 = 72\ m^{1.22}\ s^{0.61}\ kg^{-0.61}$.

1.2 Surface emitter models

1.2.1 Solid flame radiation model (ZFS, conventional)

$$\overline{SEP}_{ZFS} = \frac{f_{rad}(d)\,\overline{\dot{Q}}_{ges}}{\pi d\,\overline{H}(d)} = \varepsilon_F\sigma\left(\overline{T}_F^4 - T_u^4\right)$$

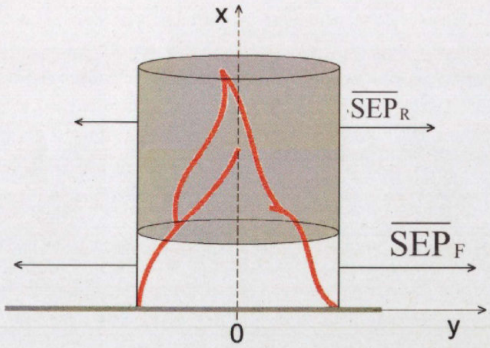


$\overline{SEP}$	[W/m²]	time-averaged *S*urface *E*missive *P*ower
ε_F	[–]	*emissivity of the flame*
σ	[W/(m²K⁴)]	*Stefan - Boltzmann* - constant
f_{rad} (d)	[–]	fraction of the combustion energy radiated $f_{rad}(d) = f_{rad,\,max}\,e^{-kd}$ with $f_{rad,\,max} = 0.35$, absorption coefficient $k = 0.05\ m^{-1}$
$\overline{T}_F$	[K]	time-averaged flame temperature
$\overline{H}$(d)	[m]	time-averaged flame length resp. -height
$\pi d\,\overline{H}(d)$	[m²]	time-averaged flame surface (surface of a cylinder)

ε_F = 0.95 (i.e. *gray* flame)
$\overline{T}_F$ = 1173 K (900 °C)
⇒
$\overline{SEP}_{ZFS}$ = 100 kW / m²
≠ f(d, fuel)

1.2.2 *Two Zone radiation model* (ZZS)

$$\overline{\mathrm{SEP}}_{\mathrm{ZZS}}(d) = \overline{\mathrm{SEP}}_{\mathrm{F}}\ a_{\mathrm{vis}}(d) + \overline{\mathrm{SEP}}_{\mathrm{R}}\ a_{\mathrm{R}}(d)$$



$\overline{\mathrm{SEP}}_{\mathrm{F}}$	[W/m²]	surface emissive power of the luminous regions o f the flame (ca.140 kW/m²)
$\mathrm{SEP}_{\mathrm{R}}$	[W/m²]	surface emissive power of the sooty regions of the flame (ca. 20 kW/m²)
$a_{\mathrm{vis}}(d) = e^{-sd}$	[–]	area fraction of the luminous flame region
$a_{\mathrm{R}}(d) = (1 - e^{-sd})$	[–]	area fraction of the sooty regions of the flame; $a_{\mathrm{R}}(d) + a_{\mathrm{vis}}(d) \equiv 1$
s	[1/m]	absorption coefficient; $s = 0.12\ \mathrm{m}^{-1}$

2.0 Experimental work

Pool fires: $1 < d < 25$ m;

n-pentane, premium gasoline,

regular grade gasoline, diesel fuel and JP-4

- ○ Instantaneous VIS-radiance structures: $0.4 < \lambda < 0.75$ µm
  [High-speed photography]
- ○ Instantaneous IR-radiance structures : $2 < \lambda < 5.6$ µm
  [Thermographic camera system with a video mixing unit, digital image analysis]
- ○ Time-averaged irradiances $\overline{E}(\Delta y / d)$: $0.6 < \lambda < 15$ µm
  [Pyroelectrical and ellipsoidal radiometry]
- ○ Meteorological data

3.0 *O*rganized *S*tructures *RA*diation *MO*del (OSRAMO II)

3.1 Basic Ideas

(1) *Reaction zones* (re):

Emitting, very hot ($\overline{T}_{re}$), homogeneous volumina of flame gas/soot particles:

they emit the fraction f_{rad} of the heat power of reaction $\dot{\overline{Q}}_{re}$

⇒ radiant exitance: $\overline{M}_{re}(d)$

(2) *Hot spots* (hs):

Intensively emitting, absorbing and transmitting hot ($\overline{T}_{hs}$), homogeneous volumina of flame gas/soot particles which are moving to the flame surface:

they emit the largest fraction of the absorbed $\overline{M}_{re}$ as heat radiation

⇒ Surface Emissive Power $\overline{SEP}_{hs}(d)$

(3) *Soot parcels* (RB):

Strongly absorbing, relatively weakly emitting and transmitting, less hot (T_{RB}), homogeneous volumina of flame gas/soot particles which are formed at the flame surface: a large fraction of the absorbed $\overline{M}_{re}$ will be transformed to nonradiant energy (*blockage effect* of the heat radiation); due to this effect the temperature of the relative cold soot particles existing in a great number, will increase for a few degree Celsius.

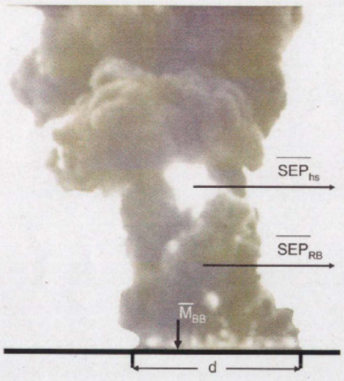
⇒ surface emissive power: $\overline{SEP}_{RB}(d)$

(4) *Fuel parcels* (BB):

Absorbing, emitting and transmitting gas volumina (BB) consisting of unburned fuel vapour and pyrolysis products. These fuel parcels exist closely above the liquid fuel surface and cause a *blockage effect* of the heat power from the flame to the fuel surface.

⇒ radiant exitance: $\overline{M}_{BB}(d)$

3.2 Basic Equations



$$\overline{SEP} \equiv \varepsilon\, M_s(T) = \varepsilon\, \sigma\left(\bar{T}^4 - T_u^4\right)$$

with

$$\overline{M}_S\left(\overline{T}\right) \equiv \int_0^\infty M_{\lambda,S}(\lambda, T)\, d\lambda$$ and

$$M_{\lambda,S}(\lambda, T) \equiv \frac{d^2\overline{\Phi}_S}{dA_1\, d\lambda}$$ as well as $\varepsilon \equiv 1 - \tau$;

$\overline{\Phi}_S$ [W] : radiation power

ε [–] : *total* emissivity

$\overline{M}[W/m^2]$: time averaged radiant exitance

$$\overline{SEP}_{OS}(d) = \overline{SEP}_{hs}(d)\;\; a_{hs}(d) + \overline{SEP}_{RB}(d)\;\; a_{RB}(d)$$

with

the radiant exitances of the hot spots (hs) and soot parcels (RB):

$$\overline{SEP}_{hs}(d) = \hat{\tau}_{hs}\left(1 - \hat{\tau}_{re}\right)\sigma\left(\overline{T}_{re}^4 - T_u^4\right) + \left(1 - \hat{\tau}_{hs}\right)\sigma\left(\overline{T}_{hs}^4 - T_u^4\right)$$

$$\overline{SEP}_{RB}(d) = \hat{\tau}_{RB}\left(1 - \hat{\tau}_{re}\right)\sigma\left(\overline{T}_{re}^4 - T_u^4\right) + \left(1 - \hat{\tau}_{RB}\right)\sigma\left(\overline{T}_{RB}^4 - T_u^4\right)$$

the *area fraction* of the hs and RB:

$$a_{hs}(d) = 1 - a_{RB}(d) \qquad , \qquad a_{RB}(d) = e^{-[d_o/d]^{a_3}}$$

the *modified effektive transmittance* of the structure elements i = re, hs, RB:

$\hat{\tau}_i(d) = e^{-k_{eff,i} d}$ where $k_{eff,i} = \dfrac{36\pi f_i(n,e)a_2}{c_2}\dfrac{c_{R,i}}{\rho_{R,i}}\overline{T}_i = 1.81 * 10^3\,\overline{T}_i m_i f_v \approx 1.12 * 10^{-3}\, m_i \overline{T}_i$

are the *modified effektive absorption coefficients* and $\overline{T}_{re}, \overline{T}_{hs}, \overline{T}_{RB}$ are the averaged *temperatures* of the structure elements i = re, hs, RB with the length-scale $\ell_i = m_i\, d$

3.3 Determination method of the parameters and results

3.3.1 Fitting along *Gram-Schmidt*-orthogonalized search directions

- Minimization of the error function of type

  $F(d, p) = \underline{f}^T \underline{f} = \min$

  due to variation of the components of the vector

  $\underline{p}^T = (d_o\ ,\ a_3\ ,\ k_{eff,re}\ ,\ k_{eff,hs}\ ,\ k_{eff,RB}\ ,\ \overline{T}_{hs}\ ,\ \overline{T}_{RB})$

  along *Gram-Schmidt*-orthogonalized search directions in consideration of parameter bounds

Here, the vector $\underline{f}$ has the form:

$$\underline{f}^T = \frac{1}{|\underline{\varphi}|}\left[\overline{SEP}_{OS}\left(d_1;\underline{p}\right)-\varphi_1,\ldots,\overline{SEP}_{OS}\left(d_N;\underline{p}\right)-\varphi_N\right]$$

N : number of measured values of the $\overline{\mathrm{SEP}}$

$\underline{\varphi} = \begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_i\end{pmatrix}$: vector of $\overline{\mathrm{SEP}}$ measured values φ_i

φ_i : measured value of $\overline{\mathrm{SEP}}$ of flames with the pool diameter d_i

3.3.2 Parameter bounds

- ○ $873 \le \overline{T}_{hs} \le 1413$ K ; $\overline{T}_{re} = 1413$ K (JP-4)

  $523 < \overline{T}_{RB} < 873$ K

- ○ $a_{RB}(d) + a_{hs}(d) = 1$

- ○ $0 \le a_3 \le \dfrac{\ln(-\ln \varepsilon_{\min})}{\ln(d_o / d_{\exp,\min})}$ with $d_o > d_{\exp,\min}$

  $\varepsilon_{\min}$ = rounding error

  $d_{\exp,\min}, d_{\exp,\max}$ = smallest, largest pool diameter for which an experimental value exists

- ○ $4.6/d_{\exp,\max} \le k_{\mathrm{eff,RB}} \le 4.6/d_{\exp,\min}$

  [It is assumed that *soot parcels* can be considered as optical thick layers with transmittance of 1 %]

3.3.3 Results: The parameters of OSRAMO II

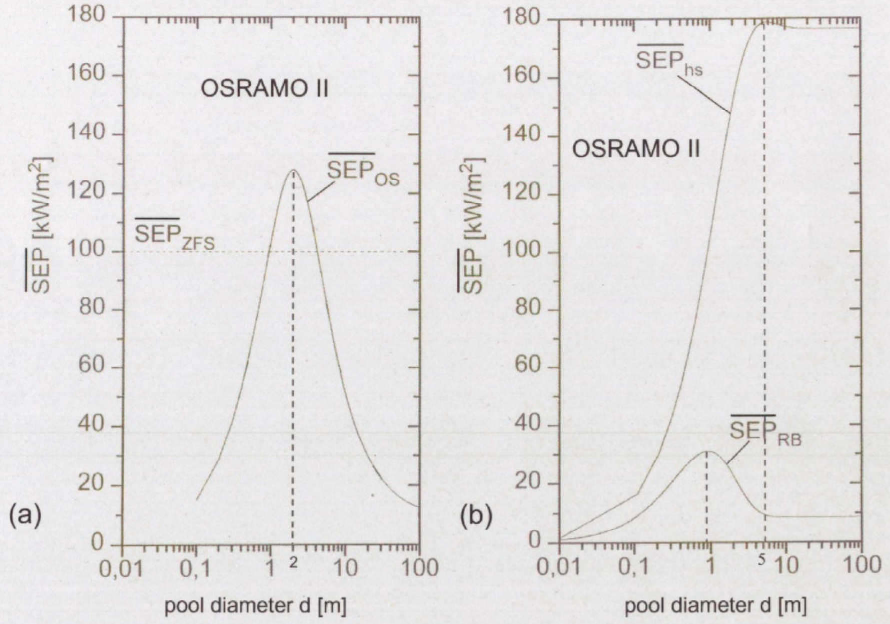
e.g. for JP-4:

$\overline{T}_{re}$ = 1413 K (1140 °C)	$k_{eff,\,re} = 0.380\ m^{-1}$	$m_{re} \approx 0.24$	$l_{re} = 0.24\ d$
$\overline{T}_{hs}$ = 1329 K (1056 °C)	$k_{eff,\,hs} = 0.404\ m^{-1}$	$m_{hs} \approx 0.27$	$l_{hs} \approx 0.27\ d$
$\overline{T}_{RB}$ = 632 K (359 °C)	$k_{eff,\,RB} = 1.035\ m^{-1}$	$m_{RB} \approx 1.46$	$l_{RB} \approx 1.46\ d$

d_o = 3.260 m

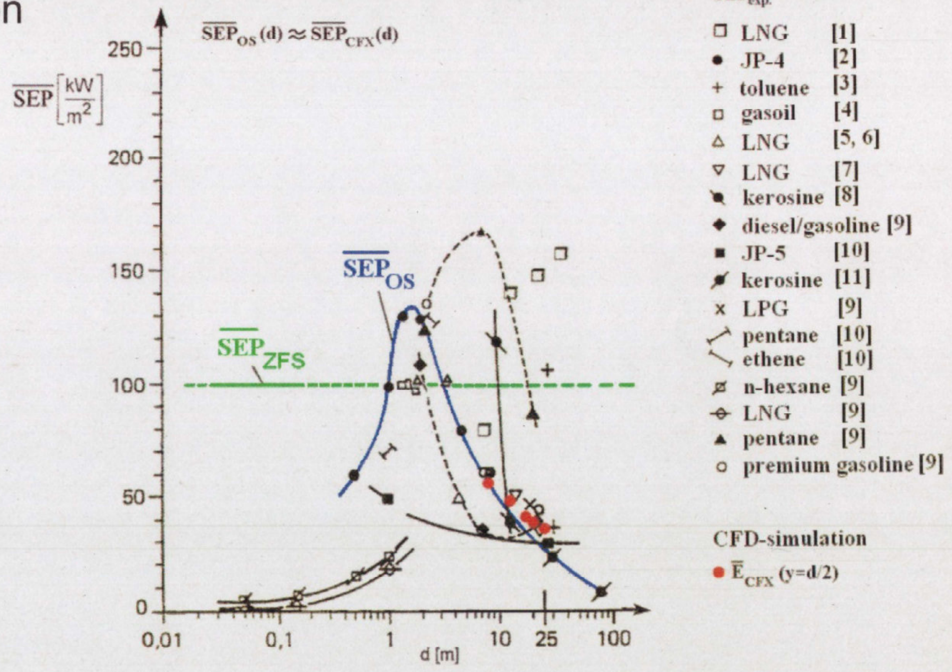
a_3 = 1.104

3.4 Calculation of $\overline{SEP}_{OS}$, $\overline{SEP}_{hs}$, $\overline{SEP}_{RB}$

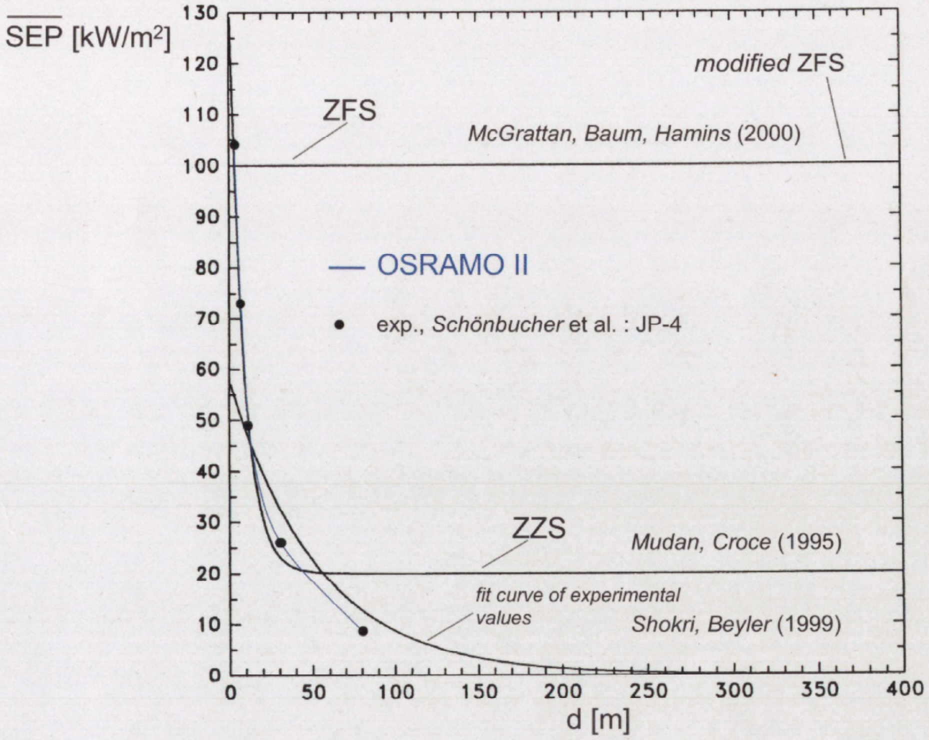


Time averaged $\overline{SEP}$: (a) $\overline{SEP}_{OS}$(d) and $\overline{SEP}_{ZFS}$; (b) $\overline{SEP}_{hs}$(d) and $\overline{SEP}_{RS}$(d) of the radiation model OSRAMO II as a function of d *for the fuels JP-4 and kerosine*

3.5 Validation



***Time averaged* $\overline{SEP}_{ZFS}$, $\overline{SEP}_{OS}$(d) of the radiation models ZFS (conventional), OSRAMO II in comparison to the *experimental* values $\overline{SEP}_{exp}$(d) as a function of p*ool diameter d* and fuel**



$\overline{SEP}$(d) for pool fires calculated with different radiation models

3.6 Calculation of irradiances

3.6.1 Assumptions and basic equation

A homogeneous isotropic and steady-state burning pool fire with the time averaged $\overline{\mathrm{SEP}}_j(d)$ at the fire surface (emitter) and the view factor $\varphi_{E,F}(\Delta y/d)$ produces at any receiver element of the area outside the fire, at the horizontal distance Δy from the pool rim, a *time-averaged* irradiance $\overline{\mathrm{E}}_j(\Delta y/d)$:

$$\overline{\mathrm{E}}_j(\Delta y/d) = \tau_a \alpha_E \varphi_{E,F}(\Delta y/d)\ \overline{\mathrm{SEP}}_j(d)$$

$\tau_a = 1 - \alpha_{H_2O} - \alpha_{CO_2}$: atmospheric transmittance

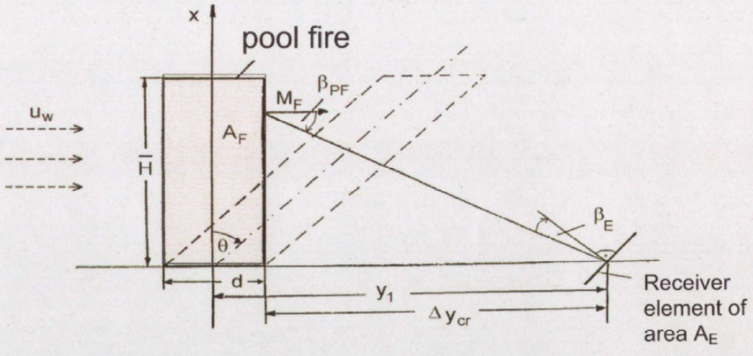
α_E : absorptance of the receiver element of area

$\alpha_{H_2O}, \alpha_{CO_2}$: absorptances of H_2O, CO_2

j = ZFS, ZZS, OSRAMO II

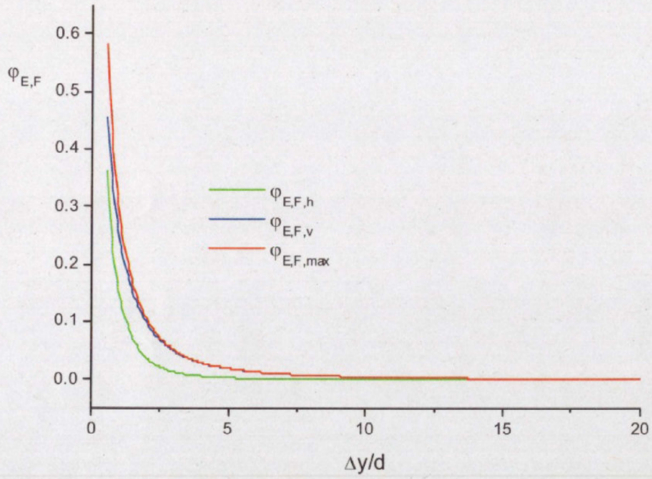
recommended : j = OSRAMO II

3.6.2 View factors



$\varphi_{E,F}$ = f (flame contour, $\Delta y/d$, relative orientation angles β_F, β_E)

$$\varphi_{E,F} = \frac{1}{\pi\,\Delta A_E} \int_{A_F} \int_{A_E} \frac{\cos\beta_F \cos\beta_E}{d^2(\Delta y/d)^2}\, dA_F\, dA_E$$



$$b = \frac{y_1}{d/2}$$

$$a = \frac{\overline{H}}{d/2} = 1.5$$

$$A = (b+1)^2 + a^2$$

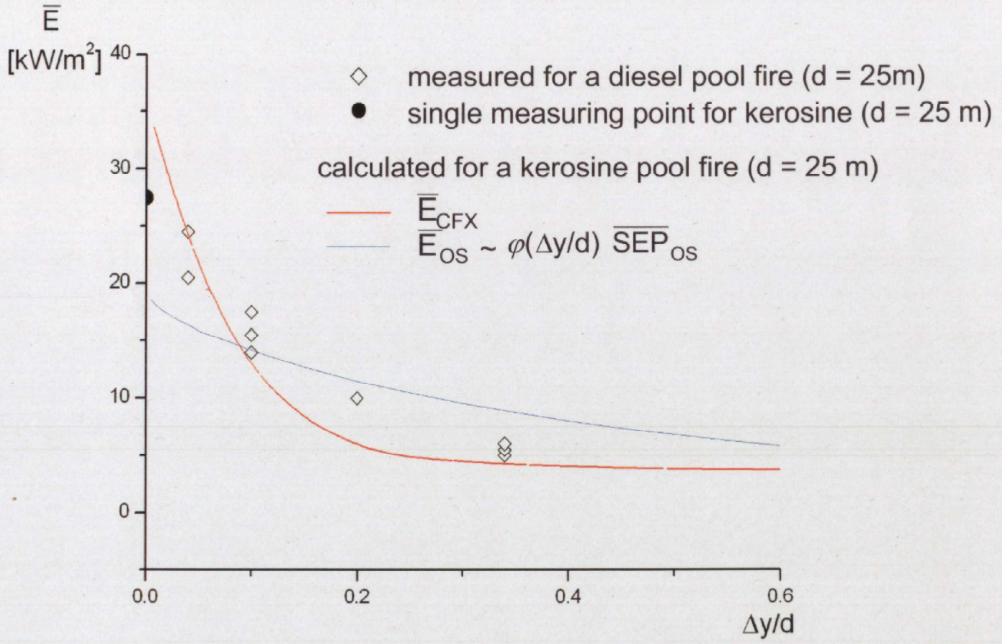
$$B = (b-1)^2 + a^2$$

$$\varphi_{E,F,max} = \sqrt{\varphi^2_{E,F,h} + \varphi^2_{E,F,v}}$$

$$\varphi_{E,F,h} = \frac{1}{\pi}\left[\arctan\sqrt{\frac{b+1}{b-1}} - \left(\frac{b^2-1+a^2}{\sqrt{AB}}\right)\arctan\sqrt{\frac{(b-1)A}{(b+1)B}}\right]$$

$$\varphi_{E,F,V} = \frac{1}{\pi}\left[\frac{1}{b}\arctan\frac{a}{\sqrt{b^2-1}} + \frac{a(A-2b)}{b\sqrt{AB}}\arctan\sqrt{\frac{(b-1)A}{(b+1)B}} - \frac{a}{b}\arctan\sqrt{\frac{b-1}{b+1}}\right]$$

3.6.3 Time averaged irradiance $\overline{E}(\Delta y/d)$



Calculated (OSRAMO II, CFX) and measured time averaged $\overline{E}(\Delta y/d)$ as a function of the relative distance Δy/d.

3.6.4 Critical irradiances

Critical irradiances E_{cr} of some technically important objects

	E_{cr} (kW/m^2)
Sensible buildings (e.g. hospitals, seniors' homes, dwelling houses, schools)	1[1] to 2
Public streets	4.5[1]
Factory buildings (e.g. control rooms, workshops)	8, 12.6[1]
Storage tanks	10, 37.8
Spontaneous ignition of wood	16 to 25
Constructions, stationary elements	18.9

[1] GER, NL, UK

Definition: E_{cr} is that irradiance at which a definite object ignites after a certain exposure time t_{cr}.

Critical irradiances E_{cr} affecting the human skin as a function of exposure time t_{cr}

Influence on the human skin		E_{cr} (kW/m^2)
Max. irradiance	t_{cr} arbitrary	≈ 1.0
Solar constant	t_{cr} arbitrary	1.3*
Pain	$10 < t_{cr} < 20$ s	4
Tolerable	$t_{ct} < 13$ s	5
Pain	$t_{cr} = 3$ s	10.5
Blisters	$10 < t_{cr} < 12$ s	10.5
Lethal dose	$t_{cr} \approx 40$ s	10
1 % lethal		25 to 32.9
Second-degree burn		27.4 to 32.9
50 % lethal		44.7 to 58.8
Third-degree burn		49 to 64.5

*extraterrestrial, at the ground: max. 0.7 – 0.9 kW/m^2, locally also < 0.6 kW/m^2

4.0 Conclusions and outlook

(1) For a realistic calculation of the heat radiation of large pool fires the extremely conservative [conventional] flame solid model (ZFS) should *no longer* be used.

(2) The semi-empirical model OSRAMO II is validated up to $d = 25$ m. It is shown that a correlation SEP = f(d, fuel) exists. The model is valid for all, e.g. *sooty* large pool and tank fires.

(3) The calculation of the view factors φ should be improved.

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(4) Unsteady (transient) CFD flame models are just at the start of development.

- New possibilities:
  - Calculation of *time-dependent heat radiation* of unsteady *pool/tank fires* as well as *gas cloud fires* and *fire balls*;
  - *Wind influence* on pool and tank fires referring to flow-, temperature- and species concentration fields
  - Evaporation and vaporization of unconfined pools
  - Formation of hot spots and soot parcels, e.g. in pool fires, resulting in time-dependent irradiances E(t).

- Improved modeling, e.g. *scale-up* of large fires
    - Simulation of the formation of pollutants: especially NO_x, SO_x, PAH, unburned hydrocarbons, soot particles and CO/CO_2
    - Different fuels, e.g. higher hydrocarbons
    - Influence of the pool diameter
    - Pool fires on *water*

- Limitations:
    - Reliable values of the properties of materials, transport coefficients
    - The extent of computational time

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(5) Requirements for future work

- Lack of measured data [e.g. SEP(d)] of larger fires, $d > 25$ m

- Lack of knowledge of the soot formation in fires of higher hydrocarbons

- Great lacks of knowledge exist for non-sooting or minor-sooting fires (e.g. methanol, acetaldehyde) as well as of large LNG fires
- Experimental work for $d \geq 25$ m should also be carried out in future
    - Time-dependent measurements of irradiances E(t)
    - Time-dependent measurements of the geometric sizes of hot spots and soot parcels

General recommendation

It is necessary and *fascinating* to carry out intensive theoretical and experimental research work *both* on small scale and large scale pool fires.

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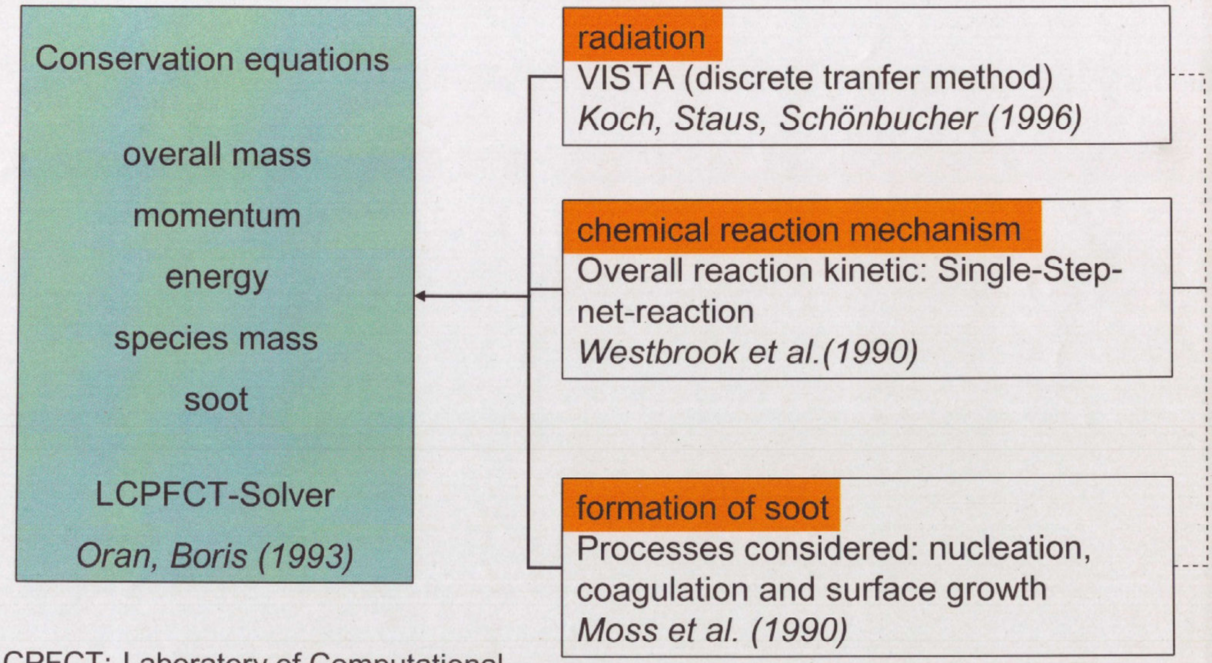
[12] Weitere Literatur auf Seite 5/32

Instationary (transient) simulation models

DNS-field model: A. Schönbucher, Th. Koch, S. Staus (1996)

d ≤ 2 cm



Conservation equations

overall mass

momentum

energy

species mass

soot

LCPFCT-Solver

Oran, Boris (1993)

radiation

VISTA (discrete tranfer method)

Koch, Staus, Schönbucher (1996)

chemical reaction mechanism

Overall reaction kinetic: Single-Step-net-reaction

Westbrook et al.(1990)

formation of soot

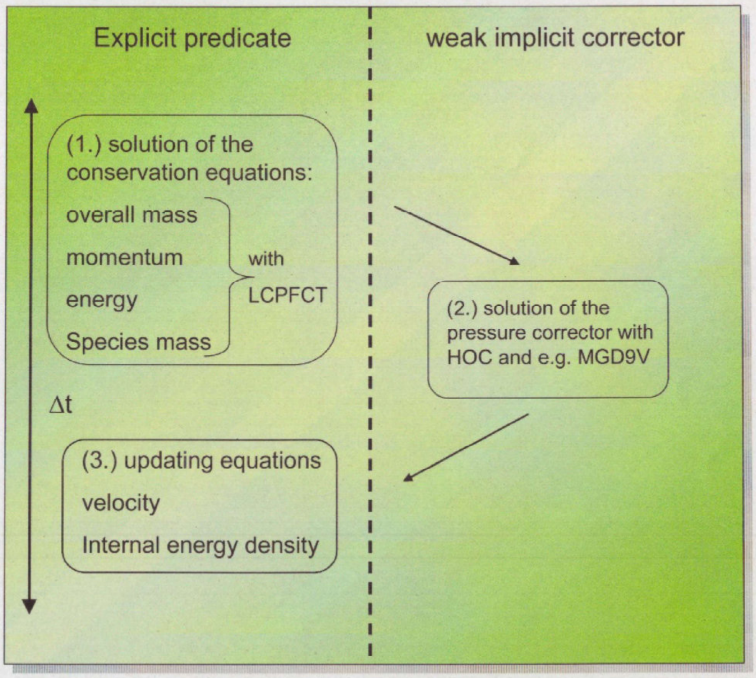
Processes considered: nucleation, coagulation and surface growth

Moss et al. (1990)

LCPFCT: Laboratory of Computational
Physics and Fluid Dynamics
Flux Corrected Transport

Extended DNS-fielmodel: *A. Schönbucher, S. Staus (1999)*

DNS extended,
d ≤ 30 cm



Explicit predicate

weak implicit corrector

(1.) solution of the conservation equations:

overall mass
momentum
energy
Species mass

with LCPFCT

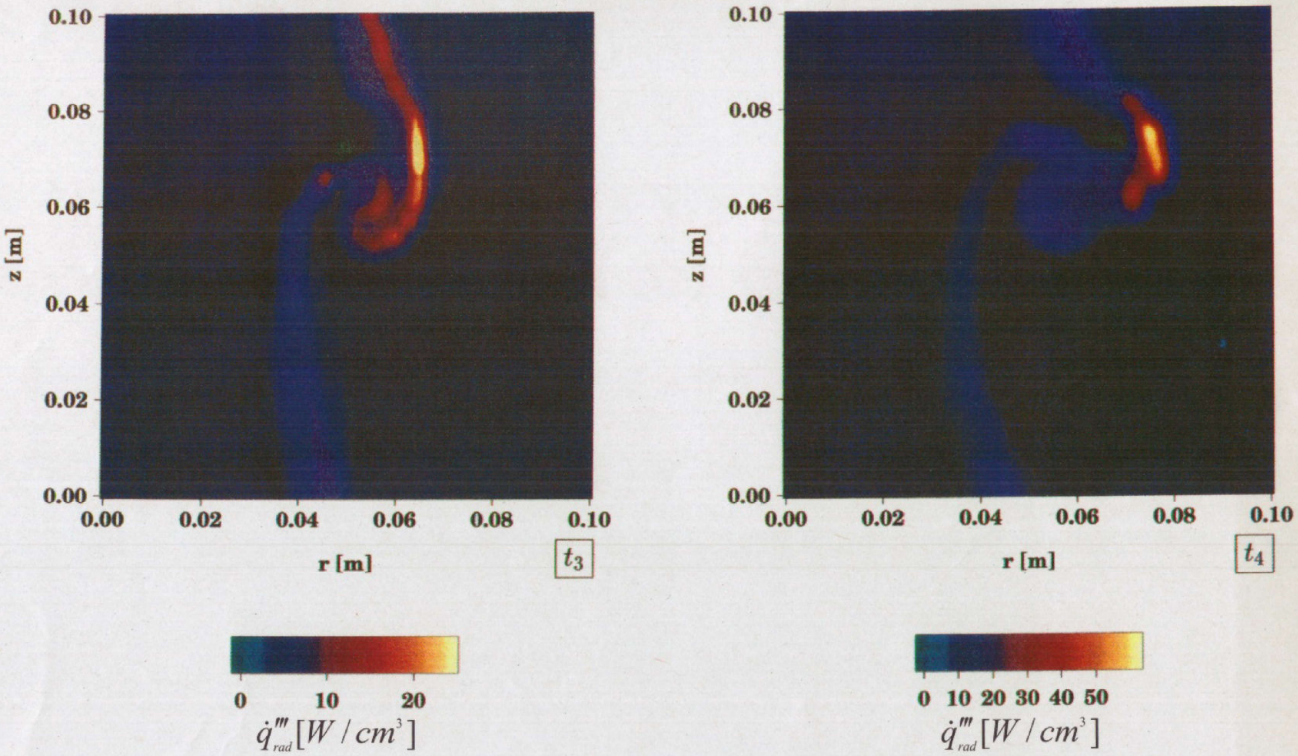
(2.) solution of the pressure corrector with HOC and e.g. MGD9V

Δt

(3.) updating equations
velocity
Internal energy density

Weak implicit correction method (*BICHOC-FCT*)

BIC : *B*arly *I*mplicit Pressure *C*orrection
HOC : *H*igh *O*rder *C*ompact
FCT : *F*lux *C*orrected *T*ransport
MGD9V : *M*ulti*G*rid-Method of P. de Zeeuw



Transient, volumetric heat radiation power at the times t_1 and t_2 in a non-premixed ethylene/air-flame (d = 0.1 m)