

# RTD software for identification of spatially localised models and data standardisation

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## Summary:

The article describes history of RTD software development at CTU Prague, and presents a review of radiotracer applications in industry of the software packages. New trends in process modelling are discussed and models are classified as either spatially undetermined (some lumped parameter models) or spatially localised (models based on CFD or combined models). Importance of spatially localised models is demonstrated on problem of irradiation (sanitation of waste water). Experimental methods using radiotracers can be used for identification of spatially localised, especially serial models. Models, which include parallel flows or "lateral units", for example spatially localised dead volumes, are more difficult for identification and characteristics of measuring instruments (first of all collimation of detectors) have to be incorporated into a model. Simplest and probably the most frequent spatially localised model assumes core-annulus flow structure. This model seems to be suitable for description of two phase flow in vertical cylindrical apparatuses, e.g. cracking units. In this case the characteristics of collimation can be simplified and expressed in an analytical form. This is not the case in more general flow structures (CFD models) and characteristics of collimation have to be evaluated numerically. Preceding analysis serves for formulation of requirement to a new generation of RTD programs. A platform independent concept is suggested (Windows, Unix): Computational core is a family of file oriented programs which communicate with a common *project file*. System is quite opened and only the format of data is to be respected by teams of developers (data standardisation). Front end processor is responsible for control of computational core (generation of script files, user friendly inputs a graphical outputs). Front end can be developed using GTK library which is implemented in either Windows or Unix OS.

## 1. Introduction

The development of RTD software have strictly followed the requests of the tracer group which had used radiotracers in industry since 1965. At the beginning of the first decade (65~75) simple systems - with one inlet and one outlet have been analyzed with simple software written in Autocod Elliot. Data registered by analog equipments could be treated for radiation decay, RC (8), detected volume (9) or tail correction and numerical characteristics (mean time and variance) of RTD could be evaluated. Simple models with lumped and distributed parameter had been used for RTD description with help of this software (1,2,3,11 and 13). At the end of this decade tracer group has started to analyze more complicated systems as apparatuses connected in series (10,14,15) or an apparatus with recirculation of input flow (4,10, and 16) or analysis of the flow from the response to the arbitrary tracer input into the system (12). Data analysis could be divided in two groups: 1) analysis of the system with no knowledge of the structure of the inside flow (so called black box analysis) or 2) analysis of the system with some knowledge of the structure of the flow (later called as grey box or parametrical analysis).

The requested software could be used not only for the evaluation of RTD but also for RTD prediction and for analysis of the methods of evaluation (e.g. study of the influence

of data fluctuation given by low values of detected counts on the precision of numerical characteristic (5) or on the evaluated parameters of the model). Algorithms for the black box analysis have led to the solution of integral equations. The orthogonal polynomials as the Laguerre functions and the Fourier series has been used for smoothing of fluctuated data (6) as well as for solution of integral equations (4,7). Several analysis have been done successfully with LF or classical FT but some have requested another sophisticated algorithms.

At the end of decade it was evident that industrial tracer applications needed two software: 1) software for black box analysis and 2) software for parameters identification and RTD prediction. Another important conclusion was that these software had to be done by professional software specialist. Since this time the new complex version of software were prepared and developed by the specialist of Czech Technical University (CTU).

## 2. History of RTD software development at CTU

First programs for the residence time distribution analysis were designed at CTU in seventies (17). There were four programs implemented on mainframe: RTD1 based upon Fourier series of Laguerre functions, RTD2 for time domain analysis, RTD3-black box identification of impulse response and RTD4-processing in the Laplace domain (using Laplace transformations for black box identification had shown to be unsuitable for most applications and was not implemented in the following RTD systems). RTD programs included also basic processing of measured responses, normalisation, calculation of moments, and correction of time courses (for the time decay of tracers, RC-correction for analog integrators, detected volume corrections, tail extrapolation etc). These programs were typically used for theoretical analysis (which algorithms are the best for identification, filtration of noise,...) and for the RTD prediction of complex production lines (18-22). Impulse responses of individual units in these lines were identified using radiotracers or approximated by simple models (e.g. series of ideal mixers). Identification of impulse responses from general input – output data were frequent and difficult problem specially in cases of data with high noise . This programming system was written in Fortran 4, and tasks were prepared as simple batches on punched tapes. For example RTD identification of an apparatus, given time courses of concentrations at inlet and outlet was specified as

```
INPUT(1)
INPUT(2)
NORM2(1,2)
ECOEF2(1,2,3)
TPOINT(3)
STOP
```

data ( $t_i, c_i$ ) for time curve 1 – inlet stream (including parameters necessary for corrections)  
 data ( $t_i, c_i$ ) for time curve 2 – outlet stream.

Second generation of the RTD software had to be written from scratch for the first programmable calculators Hewlett Packard HP9830 and HP85 in the late seventies (Basic). Several evaluations of experiments by this software have been published (e.g. 23,24,25)

In the eighties the existence of the new equipment - mainframe (IBM 370) and PC IBM XT stimulated a software project aimed at an interactive user interface compatible for either mainframe (VM OS) and PC (MS DOS). This project resulted to the library INTERFOR (INTeractive FORtran), and subroutines of this library, e.g. matrix editor, input panels, graphics, were used in the third generation of the RTD software, which is updated up to now.

RTD package consists of the three independent programs:

- RTD0 (preprocessing of non-standard experimental data: transformation of non-equidistant  $t, c$  courses,  $Z$ -transformation of  $t, c$  and  $t, Q$  courses to  $c(Z)$  at variable flow problems, time decay, decomposition of time curves to exponential or power functions /regression in selected time range/, background raise corrections, etc.),
- RTD1 (black box analysis) and
- RTD2 (lumped parameter models):

The **black box** approach (RTD1) is based on impulse responses determined from tracer experiments. Operations, like convolutions, and correlations, are performed usually in Fourier domain (FFT). Thus it is not possible to use the RTD1 system for modelling of nonlinear systems, time varying process parameters, etc.

The **gray box** approach (RTD2 - lumped parameter models-equations oriented) is obviously more flexible, however, inclusion of the experimentally determined impulse responses to the model definition is excluded.

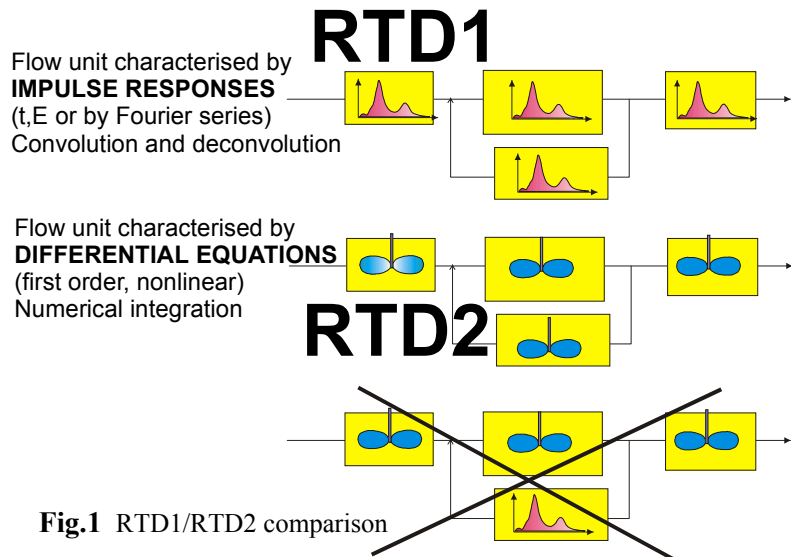


Fig.1 RTD1/RTD2 comparison

Continuing development concerned first of all improvement of numerical algorithms. Most of them are more or less standard (e.g. FFT /correlation/, numerical integration Runge-Kutta), some are unique:

- deconvolution stabilised by regularisation either in the time, Fourier or the Laguerre domain,
- identification of model parameters of mixed type (integer/real) and others.
- Characteristic feature of the RTD system consists in definition of models using a very simple language – this description can be easily modified, automatically compiled to RPN (reverse polish notation) and interpreted. It was assumed that specific models could be easily prepared by user. Flexibility of the model definition enables to include lot of specific features:
  - variable flow or variable volume,
  - axial dispersion
  - collimation characteristics of detectors,
  - heat transfer (convective transfer and chemical reactions),
  - multiple inlets/outlets,
  - heterogeneous system (particle size distribution),
  - batch systems etc.

There are also drawbacks: MS-DOS (16 bits) oriented programs RTD do not fulfil contemporary requirements for user friendliness and first of all they have limited capacity. Maximum of 20 differential equations and restricted length of model definition file is not sufficient for definition of more complicated models. Maximum 2048 time points is sometimes too small for the flow rate evaluation using cross-correlation method (FFT) and so on. Programs RTD are not portable to Unix or Linux platforms because they are tightly bound with libraries INTERFOR.

Looking back, it seems that the software concept of the first generation was the best, at least from the point of view of portability, strict modularity and simplicity. Not being pure technical reason (source programs on paper tapes) these 25-years old programs could have been transferred either to PC, or Unix / Linux without necessity to change anything. Algorithms which were used in this first generation are obviously obsolete, and impossibility of a graphical editing of time courses make such a transfer silly, however the concept was sound.

The time life of one generation of RTD programs is approximately 8 years. So it seems that the time has grown for the next generation; but it is not the time, rather CFD (Computer Fluid Dynamics) and OS (operating systems) which necessitate the radical changes. Experience shows that the first conceptual version of a new generation of RTD programs were completed in one year after the project had been launched. It took two more years to bring the system into its full strength.

Coming from history towards the future we postpone discussion of the fourth generation of the RTD system to the last chapter of this report.

### 3. RTD0,1,2 software application

Although the RTD0,1,2 software is rather old fashioned, it's great advantage is that it can be used for almost all applications of radiotracers in industry and that it is simple to use for data evaluation received from multidetector systems or from the system with variable flow or volumes, etc. RTD 0,1,2 are still used and new models for nonlinear regression have been developed. While 23 RTD models were presented in published manual [33], more than ten new models -(e.g. for the data treatment received from the so called walls detectors, for an analysis of the batch systems, or systems with variable flow or volumes), have been developed and used since that time. Applications are summarised in Table 1 for RTD0, Table 2 for RTD 1 and Table 3 for RTD2. A lot of successful applications have fulfilled requests of the tracer group in past and are successfully used at present as well.

Table 1. *RTD 0 Examples of application*

TASK	MEASUREMENT & EVALUATION	REFEREN CE
1) Steam velocity measurement Venturimeter calibration;(NZ)	Peak positions, centroid, (first moments) evaluation	[28, 33]
2) Effective volume, holdup; a) Q = constant; b) Q(t) = variable with time Waste stabilization pond (Ph; Ml) Holding tanks (Alumina industry) (Au) c) Q(l) = variable with length; horizontal rotary kiln (Cz)	a) First moment /V/Q; $\delta(t)$ b) First moment of E(z), E(t) after z transform. c) First moments,	[27] [27, 31, 33,36,39] [39, 40]
3) Parallel flow analysis, bypass, channel., a) Tank with settler - pilot plant (K) b) Ethylalcohol reactor (Cz) c) Precipitation tanks (Au) d) Holding tanks (Au)	a) rough estimation from F(t) (bypass $F^2 > 1$ ); b, c,d) decomposition by exponen. regression, background raise correction	[27, 30] [28] [41]
4) Mixing characteristic, axial dispersion	Numerical characteristic of RTD, $F^2$ ; Pe	[27]

5) Recirculation flowrate ratio	Numerical characteristics of system $E(t)$ ; relation for $T_{mean}$ and variance	Guidebook
6) Separation effect - tracer balance Cement industry -Cyclone (K)	Area below two responses; Tail correction	[28]
7) RTD	Impulse response evaluation	[27,28..]

Table 2. RTD 1 Example of application

Task	Measurement & Evaluation	Reference
1)Flowrate-velocity a)Steam velocity measur.(NZ) b) flowrate measurement (K) c) incinerator (NZ) d) small flowrates by therm.pulse	Crosscorrelation; Time delay (first moments) evaluation	[28, 33] [28] [34] [41]
2) RTD functions: E(t), F(t), $\delta(t)$ a)Fluidized catalytic cracking (Au, Fi)  b) Settling tank; waste water treatment (Cz) c) Heat exchanger (In,K) d) Evaporator (In) e)Aniline reactor (In) f) Indirect rotary dryer (In) g) Mercury removal unit (Th) h) Electron beam gas chamber (K) i) Flow invertors (Cz) j) Ohmic heater (Cz)	a)Arbitrary input response (input output needed for E(t) identification): system with recycle; black box analysis: 1)linear splines (LS); 2)Laguerre functions (LF); 3)Fast Fourier Transf. (FFT) LS  LS, FFT LF LF LS LS LS LS, LF LF	[29,33,39]  [26, 33] [35] [28] [28] [28] [28] [35] [42] [43]
3)Smoothing, damping, disturbance attenuation capabil. waste water treatment (Cz)	E(t), D(t)	[26, 33]
4)Transfer and frequency funct.; Frequency characteristics, a) waste water treatment (Cz) b) furnace for glass (Cz)	E(t), Laplace transform- f(s) Fourrier transform f(jT ); (gain ~ amplitude ratio, phase shift)	[26, 33] [33]

Table 3. RTD2 Examples of application

S Y S T E M	Evaluation	Ref.
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1) Pilot plants a) Mixed Tank (K); b) Extractor (Tl) c) Hygienization irradiator for waste water (batch system)	a) Paralell Flow (SIM+PF(SIM));SIMBMX, ' - model; b) stagnancy evaluation special model; c) Special models for batch with one or two detectors (SIMDV, SIMBMX with PF in recycle	[27] [27] [39]
2) Waste water treatment Tank of activated sludge (TAS) a) longitudinal with 30 air tubes (Ge) b) TAS with aeration turbines (Cz) c) Gold system of activation (Cz) Sedimentation tanks (Cz) Equalization unit (Cz) Equalization of variance of impurities Facultative oxidation Pond (Ph,MI)	a) RTD of water and sludge flow SIMBMX b) SIMBMX; c) Separate inputs flows with SIMBMX SIMBX with recycle (SIM+PF) Prediction by: IM+bypass;IM+rec.(PF); SIM;SIMDV;SIMBMX for variable flow	[26,33] [26,33] [26] [27,31,36]
3) Heat exchange Tubular heat exchanger (In),(K)	' -model, SIMBMX	[28,35]
4) Evaporation, dehydration a) Semi-Kestner(sugar industry) (In) b) Rotary dryer (In) c) Dehydration rotational furnace (pigment production) (Cz)	a)SIMDV+PF;bypass~parallel flow: IM(PF)+PF; b)parallel flow: SIM+SIM; c)Special model: SIM+RRDF (=Rosin Rammler distribut. of particle diameter)	[28] [28] [38,39,40]
5) Reactors a) Production of aldehydes (Cz) b) Production of aniline (In) c) FCC crackinkg (1)Au, (2) Fi)	a)(PF)SIMBMX b)parallel flow: SIM+SIM c)core-annulus model with back and cross mixing and with "wall"detectors: 1) SIMBMX+SIM with crossmixing; detector perpendicular to axis of flow; 2)SIM+SIM with crossmixing and with vertical slit collimator and excentrically located detector	[33] [28] [32] [38]
6) Alumina production (Au) a) precipitators; b) digestors; c) agglomeration d) holding tanks	RTD models used in nonlinear regression a) SIMDV + recirculation; b) SIMDV c) (SIM)PF+recycle(IM); c) SIMBMX +recycle	[38,40]
7) Electron beams gas chamber (K) a) chamber with baffles b) chamber without baffles	Comparison of CFD and LPM SIMDV SIMDV, SIMBMX	[35]
8) Disintegration effect a) hammer mill (Cz) b) drum furnace (Cz)	"Active" tracer to study techn. process:. a) rate of crushing+screening; b) rate of disintegration	[33] [37,38]

PF- plug flow;IM-ideal mixer ;SIM-series of ideal mixers; SIMBMX-series ideal mixers with backmixing ;SIMDV-series ideal mixers with stagnancy (dead volume with flow exchange)  
Au -TRACERCO Australia; Cz- CVUT, Czech Rep.; Fi- IIM, Finland; In - BARC, India;  
K- KAERI, Korea; MI - MINT, Malaysia; NZ - IGNS, New Zealand; Ph - PNRI, Philipiness;

TI - OAEP, Thailand.

#### 4. Process modelling, LPM and CFD

Residence time distribution is a characteristic closely related to the processes taking place inside an apparatus. There are two principal families of models describing these processes:

1. **Lumped parameter models** (LPM called also compartment models) taking into account only *mass balances* (continuity equations) - RTD software or DFS 4.2 PROGEPI software are examples of implementations. Flow structure is described as a flowsheet with two kinds of flow units: Ideally mixed unit, and piston flow unit (in some cases non-ideal piston flow with axial dispersion). Mass balances alone are not sufficient even for identification of the flow structure and additional information must be supplied using tracer experiments (e.g. as experimentally determined RTD).
2. **Computer Fluid Dynamics** (CFD) takes into account *mass, momentum, and heat* balances – FLUENT, CFX, COSMOS software are examples of implementation. CFD describes processes in terms of spatially localised flow units (control volumes) interconnected by mass, momentum and heat streams. This approach needs no additional information only in the case of laminar one phase flows. Turbulent flows are described using models of turbulence ( $k-\epsilon$ , RNG), multiphase flows are modeled either by using Lagrangian approach (particular and continuous phases) or pseudo-continuous phases, and so on. Though these models should be sufficiently general (in the sense, that their numerical parameters are independent of a specific case), experience shows, that the models have to be tuned using experimental data.

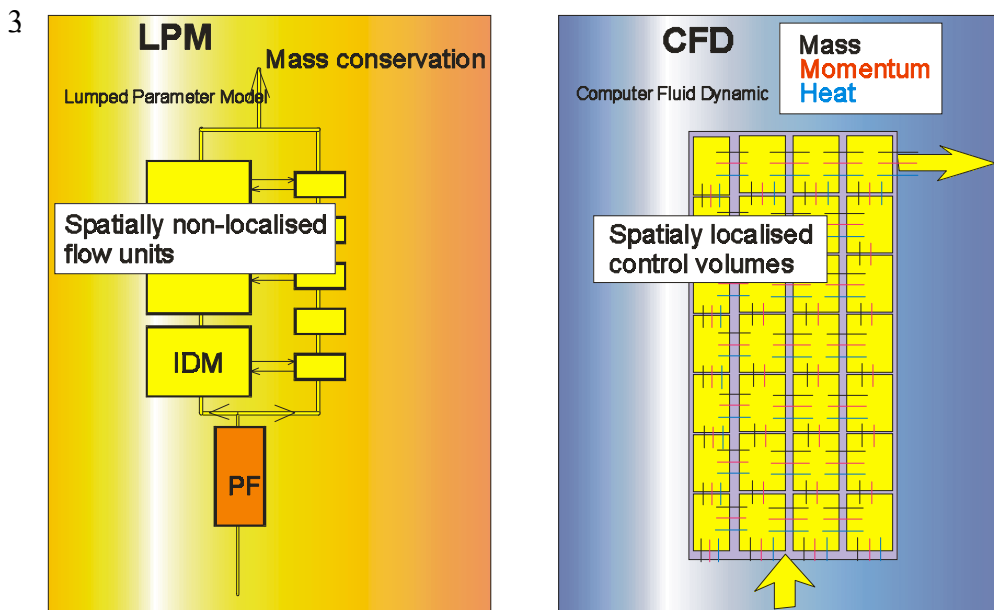
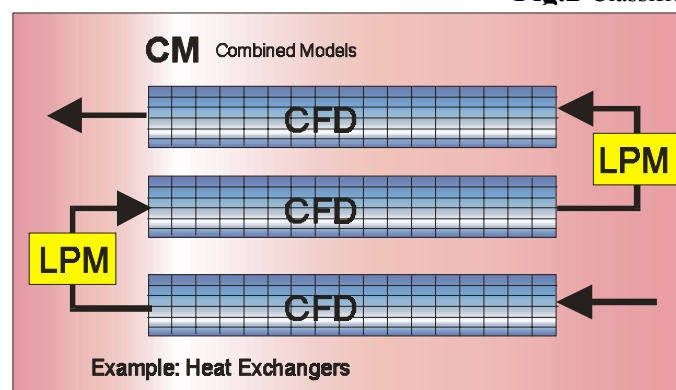


Fig.2 Classification of models

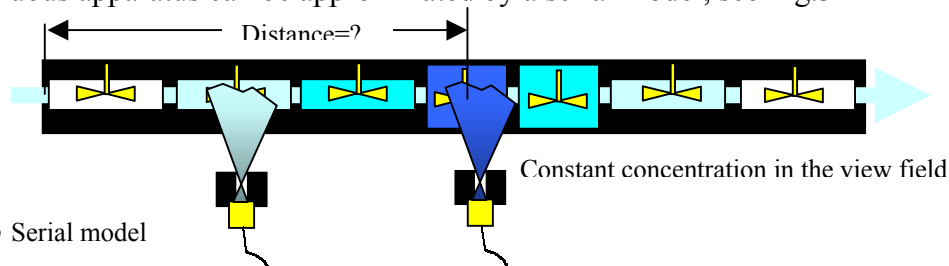




**Combined Models (CM).** There exist applications where a combination of CFD and LPM could be suitable compromise between accuracy and complexity of models. Typical example represents the tubular heat exchanger (holding tube in a pasteurisation unit), which is shown in Fig.2. While the straight pipe sections are suitable for CFD modelling (2D approximation), the difficult sections, bends, can be substituted by the LPM models of flow invertors. It seems that these combined models will be useful for many applications, and for example even Fluent (CFD packages) attempted to include some features of CM into its code (LPM of fans, heat exchangers). The method of integration of LPM used by Fluent is not very flexible, because the list of LPM is fixed, however new projects of the CM oriented software is under development, e.g. TUPLEX version 6 (Žitný R.: TUPLEX-tube and plate heat exchangers, Version 5.1, 5.2, Reference manual, CTU Prague, 1999).

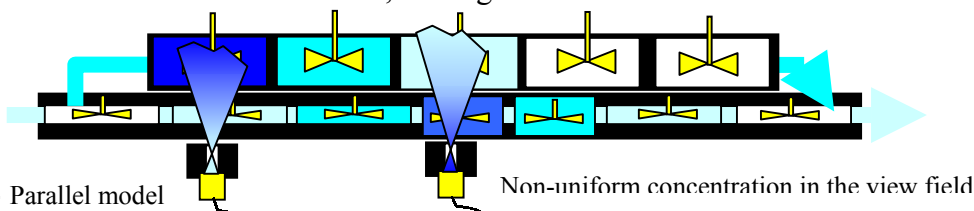
*Summary:* In principle, CFD models are more precise and more independent of experimental data than the LP models, because more balances are respected in CFD. However, CFD relies upon semiempirical models of momentum, heat and mass transfer in most of applications concerning turbulent or multiphase flows. Therefore even the CFD modelling requires at least experimental verification of predicted results (i.e. comparison with measured temperatures, pressures or composition, but in isothermal flows which are not accompanied by composition changes the radiotracers might be the only alternative). It is not only uncertainties of physical models used by CFD programs, relevant process parameters (generally speaking boundary conditions) must be also frequently determined from experiment. For example even the mass flowrate or the wall temperature of furnaces are often not known with sufficient accuracy. In this case it is possible to use radiotracers and evaluate RTD. However, e.g. the mean residence time is not sufficient for calculation of flowrate not knowing the holdup. Then it is necessary to model the process using CFD programs for several different flowrates and compare results with experiments.

This article introduces the notion of *spatially localised models*. For example all CFD models are spatially localised because position of any cell (control volume, finite element) is known. This localisation of flow need not be ensured in LPM. LPM localisation requires multiple detector technique; no principal problem are encountered when the flow field in a continuous apparatus can be approximated by a serial model, see Fig.3



**Fig.3** Serial model

All CFD models, or LPM describing parallel flows (for example annular flow) are more demanding, because characteristics of collimation have to be considered and cannot be separated from the identified model, see Fig.4.



**Fig.4** Parallel model

*Conclusion:* Spatially determined models are necessary for better description and design of processes (e.g. irradiators, see next). In these cases at least geometrical characteristics of collimators must be included into identified models.

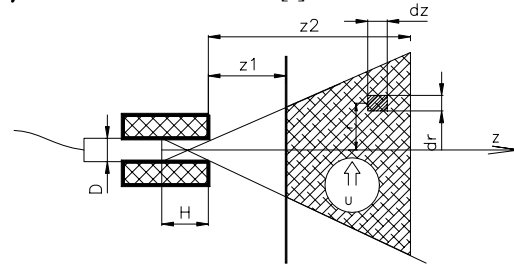
## 5. Current projects

Identification of spatially localised models – inclusion collimation characteristics into a model definition.

Core - annulus model with back- and cross-mixing, has been analysed, implemented and tested using current RTD system. The model assumes that a collimated detector is oriented perpendicular to the flow axis at a symmetry plane. A very simple geometry of collimation, and other simplifications enable to include the algorithms of collimator into the definition of model.

### Model parameters:

1. **k**-calibration constant of the wall detector
  2. **f**-flow fraction in the core region, 0-1 [-]
  3. **b**-crossmixing, 0- $\infty$  [-]
  4. **h**-backmixing 0- $\infty$  [-]
  5.  **$\beta$** -mean time  $t_2/t_1$  ratio [-]
  6.  **$\bar{t}$**  - mean residence time [s]
  7. **N**-number of mixed regions
- $\mu R$** -attenuation x Radius [-]



### Attenuation of $\gamma$ radiation

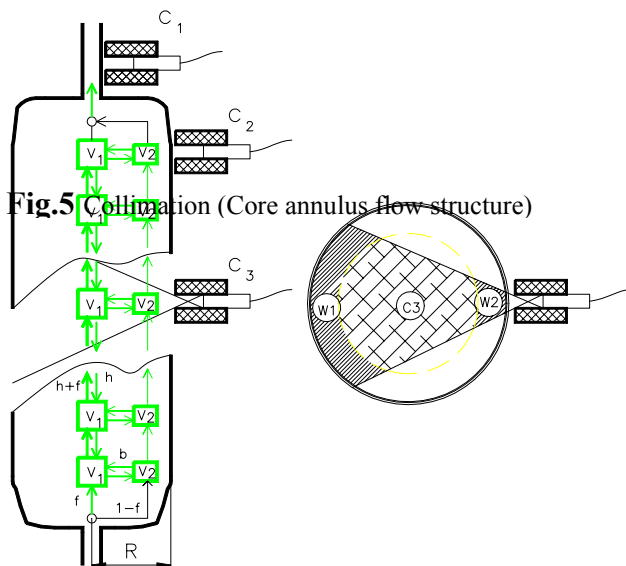
$$J = \frac{kc}{\mu^2 u} [(1 + \mu z_1) e^{-\mu z_1} - (1 + \mu z_2) e^{-\mu z_2}]$$

**J**-count rate registered by the detector

**$\mu$** -attenuation coefficient [1/m]

**u**-velocity of tracer in the layer  $[z_1, z_2]$

**c**-tracer concentration in the layer



### Spatially localised

#### Core – Annulus model

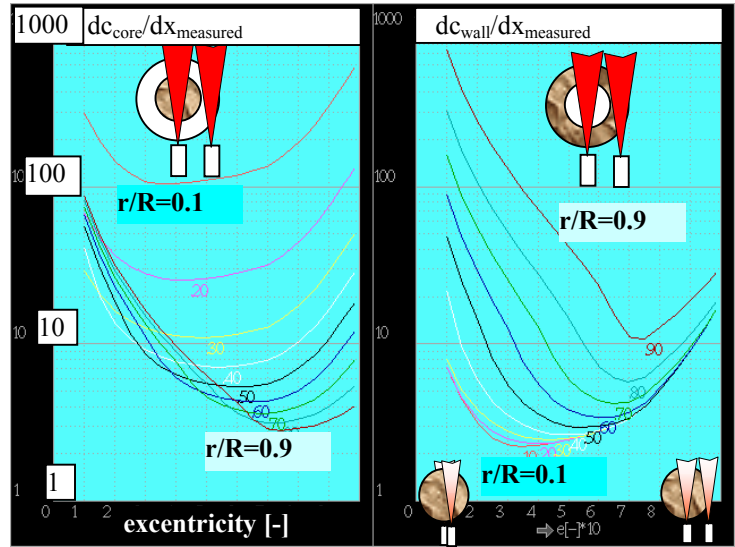
Numerical experiments proved, that it is sometimes necessary to use the multiple detector system to avoid ambiguity of the model parameters identification by comparing prediction of model with measured responses, see (32).

Similar model and similar analysis of collimator was applied to data, obtained by multiple detector system on a Fluidised Catalytic Cracking unit (FCC). The LP model of annulus-core flow was even simpler, two parallel series of mixed cells without backmixing, however algorithm of detectors was more complicated. Collimators have the form of a vertical slit, and first of all they are located eccentrically (this is necessary if the core and annular region is to be distinguished). RTD program evaluates reading from pairs of detectors, shown in Fig. 6 (cross section of cylindrical apparatus at a plane, where the two detectors were located): Annulus-core model assumes, that the concentration of tracer ( $c_{core}$ ) is constant within the core (radius  $r$ ) and equals  $c_{wall}$  within the annular ring (outer radius  $R$ ) at a given time. Reading of two detectors equipped with slit collimators is  $x_1$  and  $x_2$  (first detector is always directed towards the axis, and the second is shifted at a distance  $e$  (relative eccentricity is  $e/R$ ). Concentrations and detectors reading are related by linear relationships

$$\begin{aligned}
c_{core}(t) &= C_{11}x_1(t) + C_{12}x_2(t) \\
c_{wall}(t) &= C_{21}x_1(t) + C_{22}x_2(t)
\end{aligned}
\tag{1}$$

where the coefficients  $C_{ij}$  depend on geometry of collimators (eccentricity  $e$  between others) and on radius of core  $r$ . However, the radius  $r$  is in fact parameter of LP model, which should be identified from data  $x_1(t)$  and  $x_2(t)$ . Reliability of identification depends on sensitivity of concentrations  $c_{core}$ ,  $c_{wall}$  calculated from Eq.(1), to small changes (fluctuations) of measured signals  $x_1$ ,  $x_2$  (count rates). This sensitivity can be expressed as

$$\begin{aligned}
\frac{dc_{core}}{dx} &\cong \sqrt{C_{11}^2 + C_{12}^2} \\
\frac{dc_{wall}}{dx} &\cong \sqrt{C_{21}^2 + C_{22}^2}
\end{aligned}
\tag{2}$$



**Fig.6** Sensivity of calculated concentrations in core-annulus

Results, obtained for FCC and collimators used in experiment are presented in Fig.6. It is obvious that either too small or too large core ( $r/R < 0.1$ ,  $r/R > 0.9$ ) and similarly too small or too large eccentricity make calculation of concentrations  $c_{core}$ ,  $c_{wall}$  impossible due to noise. It is seen that for relative eccentricity of detectors  $e/R = 0.5$ , the amplification of errors will be less than 10x for dimension of core within  $r/R \in (0.3, 1)_{core}$ , and  $r/R \in (0, 0.75)_{wall}$ . Therefore only if the dimension of core is within the range  $r/R \in (0.3, 75)$  the results of identification can be considered as valid.

These two examples demonstrate the way, how the characteristics of collimators can be included into a simple LP model of annulus-core. The fact that these characteristics can be expressed in an *analytical* form follows from simple spatial distribution of concentration (there are only two regions with constant  $c_{core}$ ,  $c_{wall}$ .) and several assumptions:

- constant attenuation  $\mu$  of radiation
- effect of Compton scattering is negligible
- view factors are calculated for simplified geometry

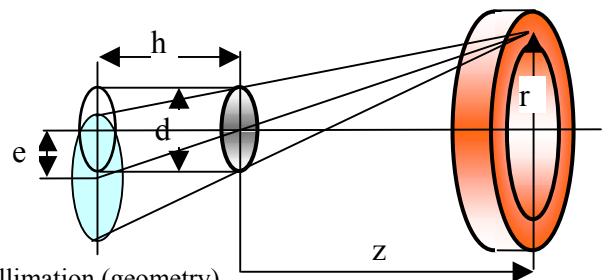
Such a procedure cannot be used in processing CFD data, characterized by quite *general spatial distribution of concentration*. The problem can be formulated like this:

- Spatial distribution of concentration of a tracer is given by a function  $c(t,x,y,z)$
- Spatial distribution of attenuation is a general function  $\mu(t,x,y,z)$ .

Remark: The functions  $c(t,x,y,z)$  and  $\mu(t,x,y,z)$  can be obtained by interpolation of nodal values (data are represented by connectivity matrix, nodal points coordinates  $x_i$ ,  $y_i$ ,  $z_i$ , and by nodal values of concentrations  $c_i$ )

- Collimator is the lead plate of the thickness  $h$  having cylindrical hole of diameter  $d$ .
- Scattering and reflections can be neglected (this assumption can be approximately satisfied if for example an energy window is used)

What is the radiation intensity detected by a perfectly shielded detector? Consider first the hole in collimator aligned with the axis  $z$  of the cylindrical coordinate system. Area of detector which is irradiated from the point  $(z,r)$  can be calculated as the intersection of two discs (the blue



**Fig.7** Collimation (geometry)

one /projection of aperture/ and the white /hole/) having radii

$$R_1 = \frac{d}{2}; R_2 = \frac{d(h+z)}{2z}, \text{ and distance of centers } e = \frac{hr}{z}. \quad (3)$$

The area of intersection of two overlapping discs equals

$$S = R_1^2 \arcsin \frac{b}{eR_1} + R_2^2 \arcsin \frac{b}{eR_2} - b, \quad (4)$$

$$\text{where } b = \frac{1}{2} \sqrt{4R_1^2 R_2^2 - (e^2 - R_1^2 - R_2^2)^2}. \quad (5)$$

Knowing irradiated area  $S$ , it is possible to calculate the fraction of radiation emitted by small element of volume ( $dV=dz dr r d\varphi$ ) which is absorbed by detector

$$dJ = \frac{Sz}{4\pi(r^2 + z^2)^{3/2}} c(t, r \cos \varphi, r \sin \varphi, z) dz \cdot dr \cdot r d\varphi \quad (6)$$

and this contribution has to be integrated within the cone  $z \in (0, \infty)$ ,  $r \in (0, z d/h)$ ,  $\varphi \in (0, 2\pi)$ . So that the attenuation could be respected numerical integration of intensity is necessary.

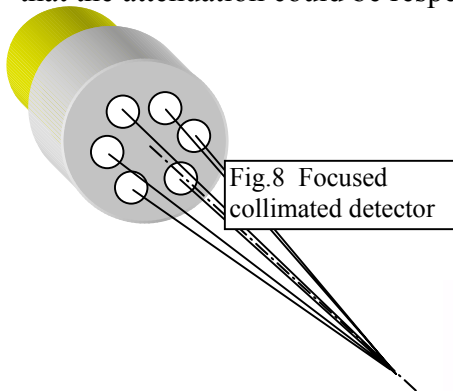


Fig.8 Focused collimated detector

Recent research concerns focused collimated detectors, shown schematically in Fig.8. The same algorithms can be used, only spatial rotations must be performed for each hole aiming towards a focus separately.

These focused collimators will be tested in experiments with continuous **direct ohmic heater**, shown in Fig.9. Numerical modeling is performed using CFD programs

COSMOS (Finite Elements) and FLUENT (Control Volumes). It is interesting to mention the amount of data delivered by Fluent for processing by algorithm of collimation: 600000 nodal point, 100 time steps. Connectivity matrix, table of coordinates of nodal points and first of all concentrations

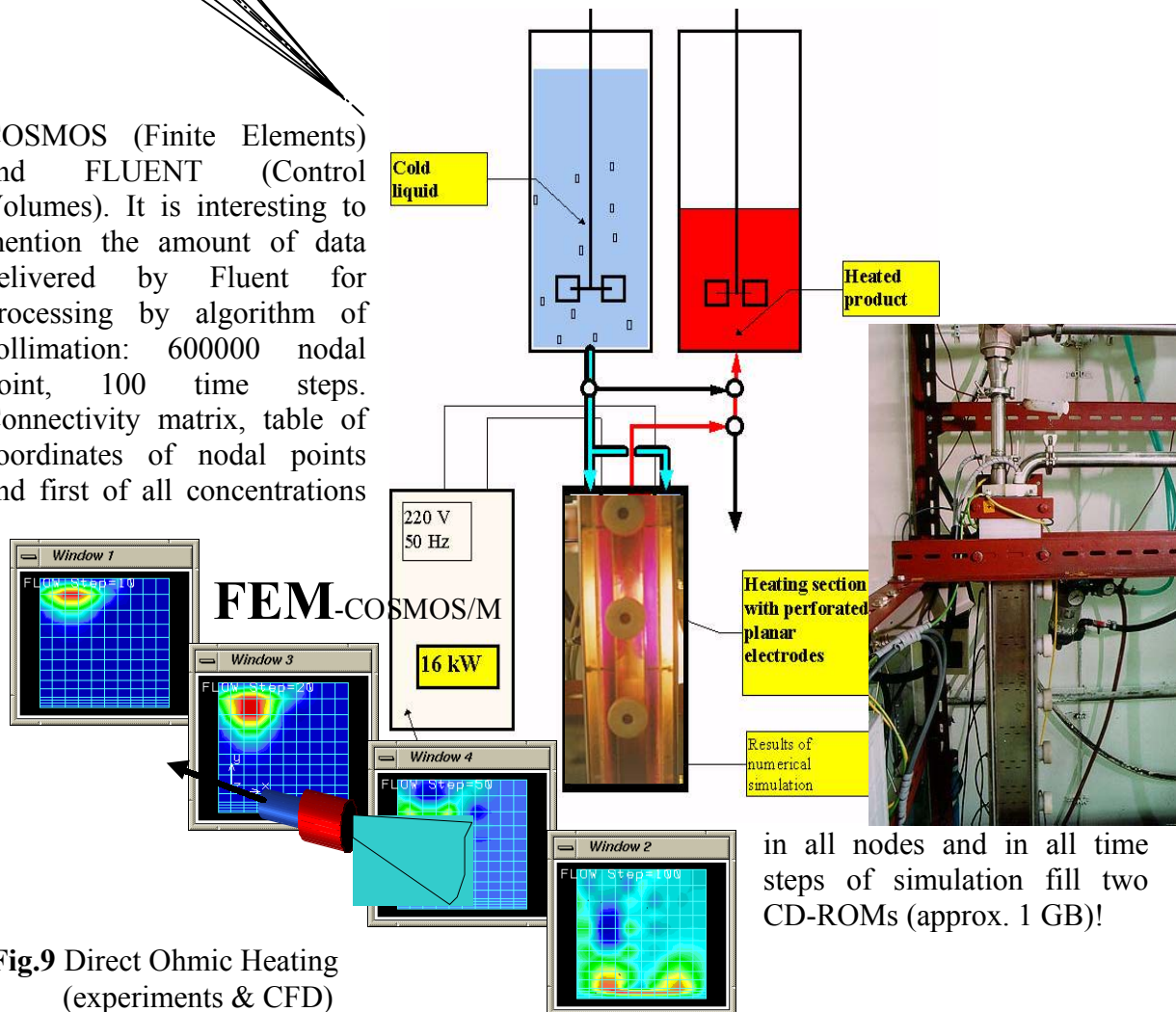


Fig.9 Direct Ohmic Heating (experiments & CFD)

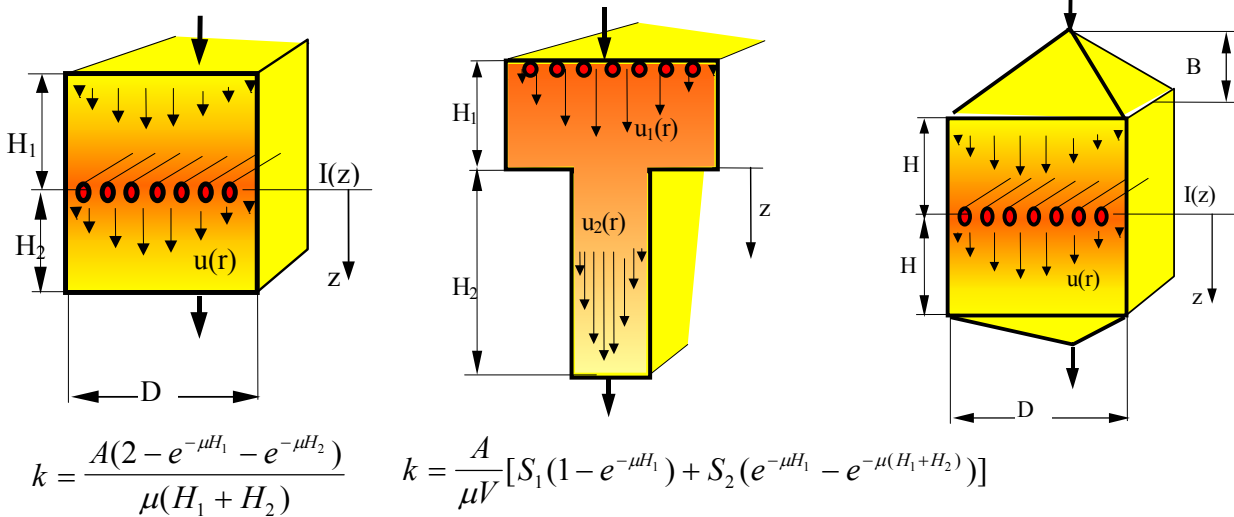
## 6. New problems and future development

**Irradiation.** Let us consider the following problem which is rather frequent in food processing or waste water treatment: how to calculate amount of energy which was absorbed by a microorganism (bacteria, virus, sponge or a mold) in material flowing through an irradiator (using radionuclides, microwaves, ultrasound or elevated temperature). The effect of irradiation can be expressed in terms of integral distribution  $W(G)$  which is the relative mass of particles having dose greater than  $G$ . Practical problem is how to estimate a portion of material which was not sufficiently treated and represents possible source of hazards. Generally speaking, the required level of dosing depends on duration and on intensity of treatment. The level of dosing depends on spatial distribution of radiation intensity and on the residence time distribution. The relationship between the residence time  $t$  and the change of dosing  $\Delta G$  can be approximated by the function

$$\Delta G(t) = kt \quad (7)$$

and the constant  $k$  can be determined for a certain class of *spatially localised* flow models, see Fig.10.

**Fig.10** Continuous irradiators (configurations which can be described by RTD)



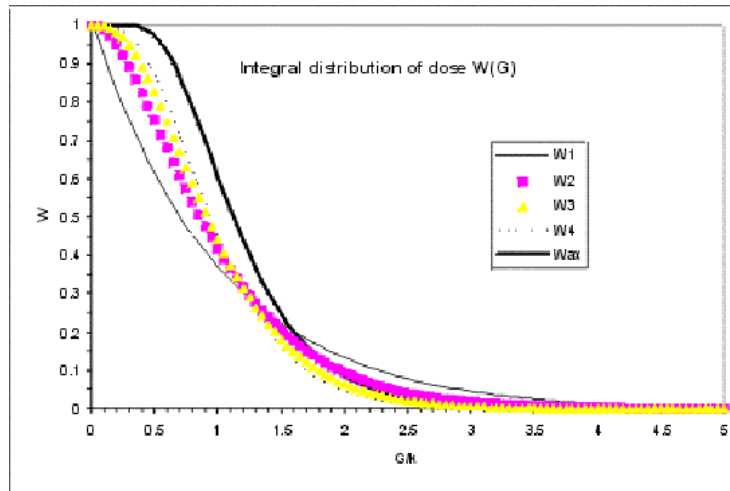
where characteristic of radiating source and absorbing media are described by

$$\dot{G} = \frac{dG}{dt} = Ae^{-\mu z} \quad (G \text{ [J/kg] is a dose, and } \mu \text{ [1/m] is attenuation coefficient).} \quad (8)$$

In these cases it is possible predict the integral *distribution* of dosing  $W(G)$  at the outlet of irradiator given the same characteristic  $W_0$  at the inlet stream and the residence time distribution of the apparatus. This relationship has the form of integral equation

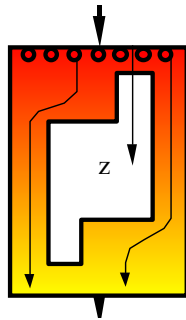
$$W(G) = \int_{-\infty}^{\infty} W_0[G - \Delta G(\tau)]E(\tau)d\tau \quad (9)$$

where  $E(t)$  is  $t$  residence time distribution of irradiator. It is assumed, that the irradiator operates in steady state, and the distribution of dosing  $W_0(G)$  is time independent at inlet. Preliminary results corresponding to simplest case when the initial dosing is zero, are shown in Fig. 11



**Fig.11** Integral distributions  $W(G)$  according to Eq.(9) for impulse responses  $E(t)$  of series of ideal mixers (mean RT =1, N=1,2,3,4) and for dispersion model with open ends and Pe=10 (mean RT=1).  $\Delta G(t)=kt$ .

There are situations, where this concept can not be used, e.g. the flow arrangement shown in Fig.12. In such a case the CFD approach seems to be the only solution. However, even if it is not possible to use the previous concept based on the residence time distribution  $E(t)$ , a spatially localised LP model enables calculation of the distribution  $W(G)$  numerically. In other words: It is necessary to use spatially localised models and it does not matter if they are CFD or LPM.



**Fig.12** Irradiator (example of flow structure when  $E(t)$  is not sufficient for calculation  $W(G)$  )

Summary: This is only an outline of the problem, which is rather broad and not fully understood yet (results presented here are preliminary and have not been published). Even the simple integral Eq.(9) is only a hypothesis, and generalisation to the time dependent distributions  $W(t, G)$  is rather complicated. Nevertheless, theoretical and experimental research is worth while such effort, because it concerns many new applications.

## 7. Software projects, portability, and standardisation

Concept of the fourth generation of RTD programs is based on the following principles:

- Computations will be performed by *separated programs*, which are independent of operational system (more precisely their source code /ANSI C or Fortran/ can be compiled without any changes under Windows, Linux, Unix or Mac operating systems, without any reference to a specific hardware or libraries).
- All inputs and outputs will be *file oriented* (ASCII files). Data file management assumes also internet links, therefore the processing can include models from different resources.
- Computational programs will be started from a *script file* (including definition of data)

This part of RTD programs and suggested structure of data file is shown in Fig. 13

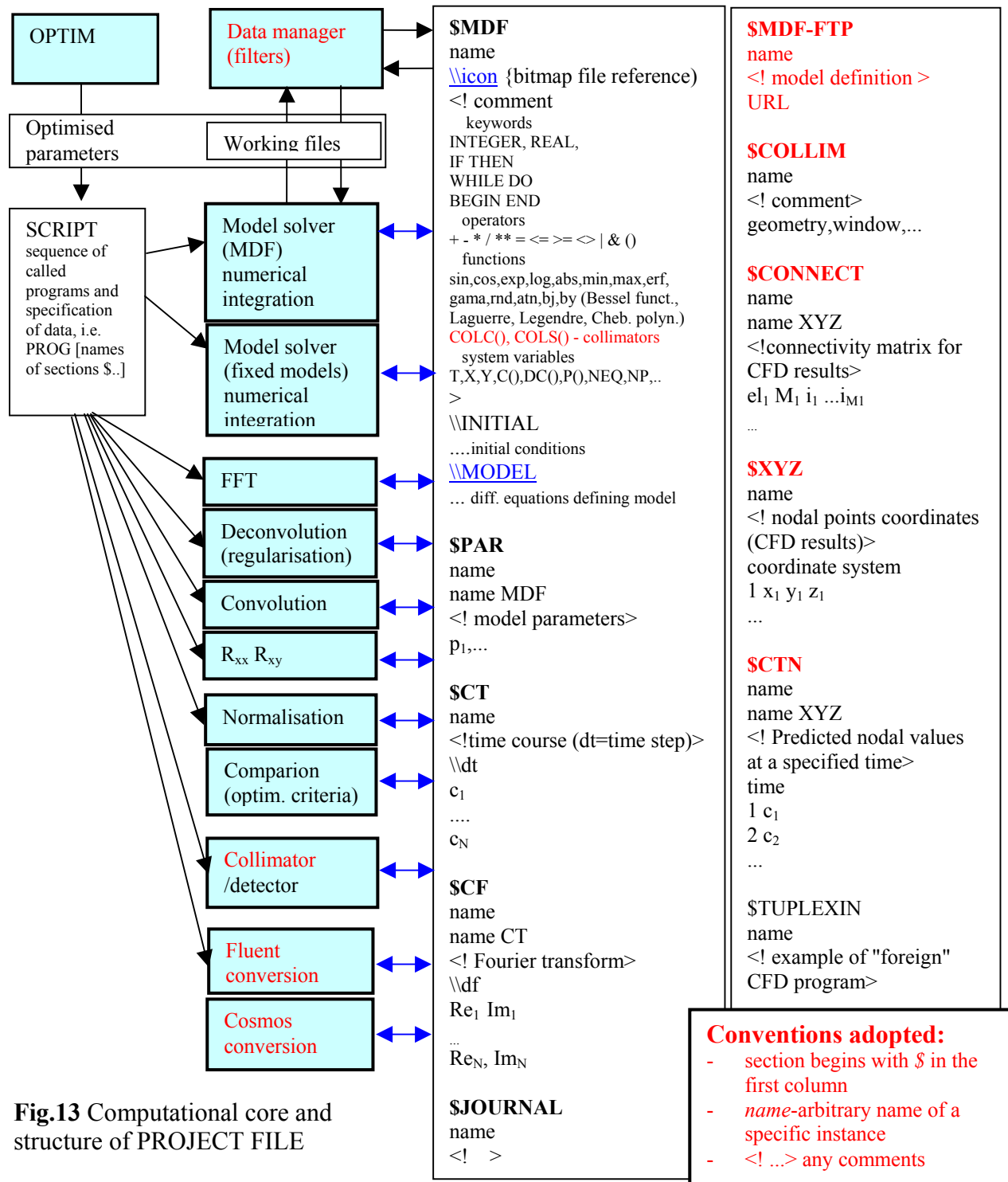


Fig.13 Computational core and structure of PROJECT FILE



The diagram is far from being complete, and the list of operations as well as the data sections could (and should) be extended at least to the level, corresponding to the current version of RTD programs. However there are also some new features:

- Besides the editable models (defined by MDF /Model Definition Files/), it is useful to define frequent or on the other hand very complicated models as *fixed*.
- Simple language and standard functions used for MDF are preserved, only a family of functions defining *collimators* is added. This is because the programming of collimators is rather complicated.
- Seemingly minor change is the possibility to include arbitrary number of models (MDF sections) into a project file. In current RTD programs the project file contains only one model (MDF), and experience shows, that this is the reason, why the idea of a single project file is not utilised (and several project files are typically used for solution of a project).
- Most of changes concerns CFD: modules for transformation of the input / output files of CFD programs, and new sections describing CFD data in a standard format, which is suitable for processing by modules of detectors (collimators).
- The structure envisage also processing of distributed data (for example models, developed and updated by different groups).

Lot of discussion concerns the following questions:

- Which language? Current version of RTD is written in Fortran77 and most of its source code can be used also for the new generation. However, Microsoft does not continue in the Fortran compilers development (the last compiler, Power Fortran, was sold to DEC). From this point of view it seems to be better to convert and adapt the current Fortran source code to the C language.
- Is it better to use just one big ASCII file for a project instead of several smaller files? The suggested idea of single common project file has been introduced in the current generation of RTD programs. Differences are small: The project file is not an ASCII but a binary file and the first section serves as a directory of all the following sections (called "matrices", this name is heritage of Interfor, which was intended mainly on interactive processing of matrices in finite element method).
- Other question: Is it better to transfer all data between computational programs and the project file via a data manager (filter, backup, undo, internet access) or directly, see the blue horizontal arrows in Fig.13?

Considering pro/cons we arrived to the following conclusion: Single common *project file*, *direct access*, and data manager in line with the other computational programs.

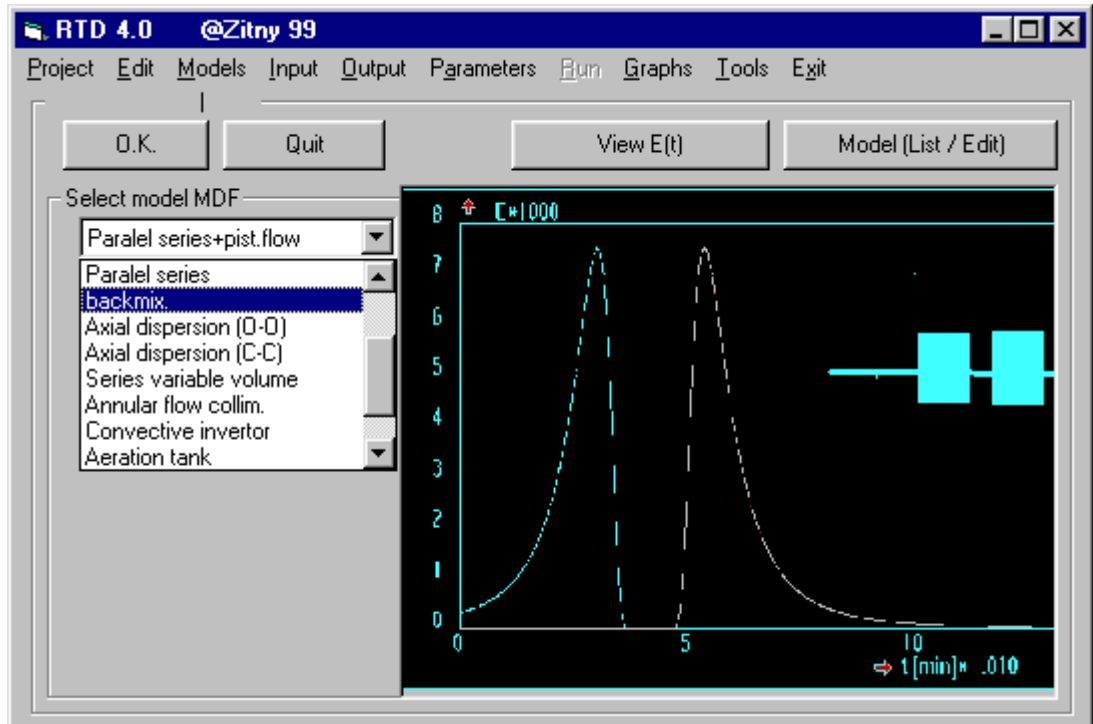
This fully portable part can be developed step by step, just adding new programs to the package. The independence of computational programs is a good platform for cooperation of different groups. It could be possible to include into the package *any program*, the only restriction is the structure of the data file described above. However, this structure is flexible and any new section can be included (an example is the section \$TUPLEX for quite a specific program). Adding such a new definition of section would not have any influence upon existing programs.

This core of the RTD system will be functional at any stage of development, however without graphical outputs and interactive inputs its applicability would be very restricted.

- Project assumes that all operations which are more or less OS/platform dependent, i.e. graphics and interactions, will be designed as an separate part, Front End of the computational core (shell of the computational programs, data manager and the project file). This shell has to generate the script file defining the sequence of processing. The

"smallest" version, designed for the program MODEL, should comprise the following steps:

- Menu of models MDF in a project file (icons of models are specified as bitmap in the project file. Icon is a schematic diagram of model topology and typical impulse response).



- For selected model a Form is to be submitted (for specification of operands and methods of integration - names of sections, containing inputs and outputs, parameters of model)
- Submit an editor of "sections" or a form enabling modification of data specified in the previous step (in fact any text editor can be used);
- Run calculation (start the generated script file)
- Submit Form for specification of graphical outputs (names of curves, labelling, colours and so on)
- To draw graphs in arithmetical coordinates with possible zooming.

Taking into account application of CFD programs and uncertainty of further evolution or spread of operating systems, this front end should be developed simultaneously for Windows and Unix/Linux. A problem represent graphs, menus and forms, which are already implemented in slightly different forms under Windows and Linux. To reduce the effort in preparing the front end a suitable library should be selected – a possible choice is GTK library, but it is still an open question. Relaxing the compatibility requirement it is possible to use e.g. Microsoft Visual Studio 5. for preparation of the front end under Windows with ease.

Suggested concept of a new generation of RTD programs relies on the long time experience with RTD systems and preserves those ideas and algorithms which proved oneself. Project should anticipate gradually changing paradigma of software design, which is discussed especially in CAD: Quality of program is not given by the amount of buttons, icons and by very sophisticated tools trying to perform lot of functions (which are often not necessary), rather by simplicity, reliability, and transparency. An important point is the possibility of cooperation of independent groups in the system development (*open system*).

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