PROGRAM COMPLEX FOR AUTOMATION OF A COMPUTER EXPERIMENT IN PLASMA DYNAMICS OF A JET DISPERSE SYSTEMS

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ABSTRACT

The problem-oriented program complex for Eulerian and Lagrangian simulation of one-phase and heterogeneous plasma jets is briefly described. Main attention is paid to its computatianal characteristics and input language of the problems formulation.

INTRODUCTION

Optimization of plasma technologies of powder material processing may be achieved only by further progress in study of the interphase momentum, -heat and mass transfer occuring in a high temperature jets of complex gas composition with dispersed admixtures. This may be provided only by formulation of the complex investigations including the computational experiment based on either Lagrangian or Eulerian simulation of a dust-laden flows.

The available models of high-temperature one-phase and dusted jets, based on the Eulerian and Lagrangian descriptions of the inertia particles, need a mutual comparison and further development taking into account some peculiarities [1] of plasma processing of powder materials, including plasma spraying. They are *(i)*--different regimes of jet flow, including different degrees of turbulence and its scales, *(ii)*--wide spectrum of particle materials to be sprayed and their different granulometric composition, *(iii)*--the particle loading effect, *(iv)*--polydispersivity, *(v)*--multicomponentness, *(vi)*--turbulent diffusion of admixtures, *(vii)*--effect of stochasticity of particle injection on its transverse spreading in a cross-sections of jet, *(viii)*--effect of condensed phase on the carrying flow turbulence structure, *(ix)*--effect of a probable evaporation of the material on a dynamical and thermal nonequalibrium, *(x)*--significant relationship between thermodynamicaly and transport properties of the gas flow, *etc.*

At the present time, however, testing and mutual comparison of the available models is difficult to be made, since the appropriate computer programs have no unified base, they are narrow specialized in their functions, and realize numerical algorithms different in their accuracy. Many difficulties may be eliminated by using the problem-oriented computational technology to automize the numerical analysis of various models in plasma dynamics of jet dispersed systems [1,2].

STRUCTURE OF THE PROBLEM-ORIENTED PROGRAM COMPLEX

When developing the fundamentals of the computational technology to simulate the flows of the boundary layer type, we proceeded from minimum requirements to their mathematical description, i.e. we did it on the basis of plane or axial symmetry and closeness of the boundary-value problems.

Analysis of variables and parameters Ψ_σ entering the description of an arbitrary boundary-value problem allows the set Ψ_σ to be subdivided into the following subsets: 1) $\Psi_0=\Psi_{01}\cup\Psi_{02}$ is the union of set Ψ_{01} of external varying physical constants and set Ψ_{02} of physical complexes uniquely represented as a functions of parameters of the set Ψ_{01}; 2) Ψ_1 is the set of known variables being analytical or tabulated functions of spatial coordinates (if a problem is nonstationary, variables of the set Ψ_1 may depend on time); 3) Ψ_2 is the set of unknown variables (required functions), obtained by the solution of the boundary-value problem; 4) Ψ_3 is the set of additional variables being the functions of variables of sets Ψ_k, $k=\overline{0,2}$.

The above-mentioned subdividing of the set Ψ_σ allows a rational structuring of the program package, an effective arrangement of the computational process and co-ordination of the input language with individual moduli of the package.

Whatever physical content and peculiarities of the flow under study, most problems may be described by the system of nonlinear second-order equations, which probably includes the first-order equation too. Formally, this system may be represented as

$$L_i[\varphi_i] = \sum_{j=1}^{N}\sum_{k=1}^{2}\sum_{l=1}^{n_{ij}}\sum_{m=0}^{2} L_m^{(j)}\left[f_0^{(j,k,l)}, f_1^{(j,k,l)}, f_2^{(j,k,l)}, \varphi_i^{k-1}\right]=0,$$

$$i=\overline{1;n},$$

where N is the number of different types of elementary differential operators forming the set Ξ; $\varphi_i\in\Psi_2$ is the so-called leading variable of the i-th equation of the boundary-value problem; $f_s^{(j,k,l)}$, $s=\overline{0,2}$ are, respectively, the coefficients of the first, second and third levels of the j-type elementary differential operator, being the functions of variable sets Ψ_i, $i=\overline{0,3}$; n_{ij} is the number of inputs into

Table 1. The basic operators of the problem-oriented language for formulation of the boundary-value problems

No.	Title of the govening operator of language	Declaration/defition of the:
1	**PROBLEM**	Problem title and commentary
2	**COORDINATES**	Coordinate system to be used
3	**CONSTANTS**	External varying parameters (Ψ_{01})
4	**COMPLEXIES**	Physical complexes and criteria (Ψ_{02})
5	**KNOWN VARIABLES**	Distributions of known variables (Ψ_1)
6	**UNKNOWN VARIABLES**	Variables to be determined by the solution of boundary-layer problem (Ψ_2)
7	**GROUP VARIABLES**	Variables corresponding to a substances divided on given number of groups
8	**TRANSFERRED SUBSTANCES**	Variables corresponding to a passive substances to be transferred in the computed field
9	**LAGRANGIAN PARTICLE**	Initial conditions of a single spherical particle to be studied in the computed fields of the velocity and temperature of the carrier gas flow
10	**TABLE FUNCTIONS**	Reference tabulated functions
11	**TABLE CONSTANTS**	Reference table-listed constants
12	**CALCULATED VARIABLES**	Calculated (auxillary) variables (Ψ_3) used by the concrete model
13	**VELOCITIES**	Variables determining the convective velocities
14	**OUTPUT VARIABLES**	Variables are to be the final result
15	**EQUIVALENCE**	Equivalent variables of the problem
16	**DOMAIN**	Geometry of the domain to be computed
17	**EQUATIONS**	Differential equations entering the concrete boundary-layer problem
18	**SOURCES**	Source terms in the right-hand part of the equations of the problem
19	**INITIAL CONDITIONS**	Initial conditions for all variables of the set Ψ_2
20	**BOUNDARY CONDITIONS**	Boundary conditions for all variables of the set Ψ_2
21	**BOUNDARY LAYES**	Variables for the boundary-layers of finite thickness are to be determined
22	**NET**	Declaration of the computing net
23	**ERRORS**	Criteria of an iterations' convergence
24	**NUMBER OF CYCLES**	Number of sub-iterations of individual equations at general iteration cycle
25	**NUMBER OF ITERATIONS**	Limiting number of cycles during the process of general iterations for the fixed cross-sections of the flow
26	**RELAXATION**	Parameters of upper/lower relaxation

the i-th equation of the j-th type operator, k being the fixed parameter. When $k=1$, the form of inputs of the leading variable into the term under consideration is nonimportant; when $k=2$, the leading variable φ_i enters multiplicatively into the s-th level coefficient.

The interface user - program complex is supported by a specially elaborated input language including a finite set of phrases, each corresponds to a definite stage of the boundary-value problem formulation or prescribing the information required for the control of a computing process (see Table 1). With this approach the solution of any problem is subdivided into two stages.

First, full definition, adjustment and generation, if necessary, of the moduli of the program package are realized following from the description of the specific mathematical model using the input language of the problem formulation. Besides, special service tables used by computer programs at the stage of computations are created. They include problem syntax, structure of the partial differential equations and of boundary conditions, topology of the computed region, *etc*. As a result, the program based on the algorithmic language *FORTRAN* is generated which maximally takes into account the characteristic features of the problem under analysis. The functions incorporated at this stage are fulfilled by a special **PREJET** program.

Second, a necessary series experiments is performed, and the computation results are analysed. If thereby, it is expedient to correct a physico-mathematical model we shall return, after introducing some appropriate variations in the problem formulation, to the first stage again.

CHARACTERISTICS OF THE COMPUTING METHOD

Computation of an arbitrary flow of the boundary-layer type is performed by marching method from a section to section. Each cross-section to be calculated represents a totality of the right (output) edges of the column of control physical volumes *(CPV)* in a transversal direction of the flow, while for the set of left edges, distribution of the varibles Ψ_σ taking part in the problem formulation are assumed known.

The computational method realized in the package of applied programs *(PAP)* is based on the finite-difference method. Its realization applied to our case is characterized by following peculiarities: 1) conservativity over the all substances to be transferred at both integral and local levels; 2) possibility of taking into account the direction of flows of substances transferred, *i.e.* use of the so-called finite-difference approximations oriented upstream; 3) use of Neuton-Raphson-Kantorovich quasilinearization method to overcome computational difficulties related to possible nonlinearity of equations; 4) making an appropriate number of nonlinearity iterations during which the differential equations entering the problem are successively scanned; 5) taking into account the increase in boundary layer thicknesses (dynamical, thermal, *etc.*) in the iteration process. All the peculiarities listed above allow for the second order of approximations in space coordinates and the first order in time.

PROGRAM JETS

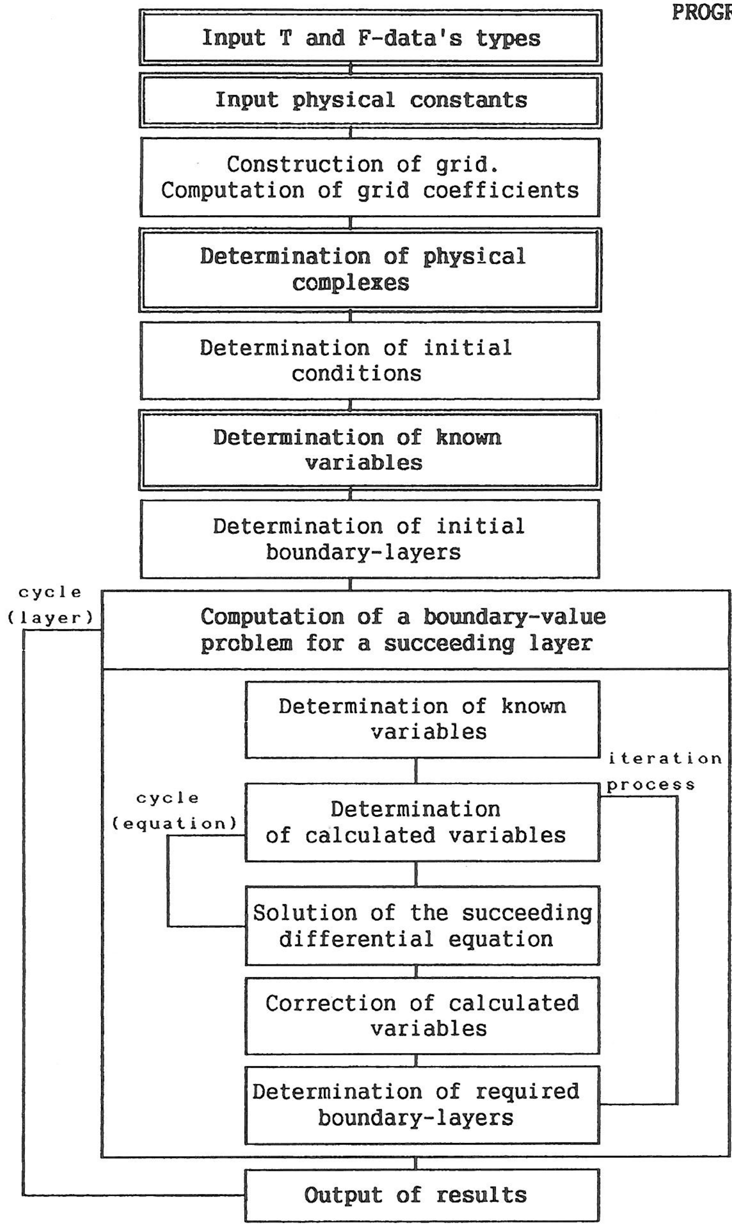

Fig.1. The principal block-diagram of the numerical solution of arbitrary flow of the boundary-layer type.

The *PAP* presented herein provides for an automatic generation of the program confirming to a physico - mathematical model of the flow under study. Fig. 1 displays the extented block-scheme of the computer program generated especially for a specific model. The computational blocks within the double-line frame state to the probable absence of the corresponding sections in the problem formulation, and, consequently, of the program moduli therewith formulated.

A basic computing core of the input program is rather universal. Its volume and set of generated subroutines are only varying due to a number of variables taking part in the mathematical description of the model, their distribution in types as well as complicated analytical dependences, used to determine them. The program becomes independent of the boundary-value problem under investigation (first of all, of the number of differential equations as well as the length and quantity of elementary differential operators *(EDO)* entering each of them) due to a special transformation of equations and boundary conditions into the 1d files of the linear structure with a variable length of records generated by the *PREJET* program. These files store full information on the equations we are solving here and on the representation of them in terms described in the corresponding sections of parameters and variables entering the problem formulation.

CONCLUSION

The program complex developed by the authors provides the program generation for a specific Eulerian physico-mathematical model of flow the boundary-layer type. This makes it possible the mutual comparison of different models describing a specific plasma flow based on the common problem-oriented software as well as to verify them experimentally and to interpret the obtained data more correctly.

Besides, due to the presence of the generation function in package of applied programs, one can start to creating the bank of programs or, in fact, the bank of the models of different flows. This possibility of the presented *PAP* is used by us at computer-aided design of plasma spraying and related technologies.

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