IMPLEMENTATION of DIFFUSION in the CESAM CODE

DIFFUSION of CHEMICAL ELEMENTS

- General diffusion equations of chemicals (Lagrangian form)

$$\frac{\partial x_i}{\partial t} = \frac{\partial F_i}{\partial M} + \left(\frac{\partial x_i}{\partial t}\right)_{\mathrm{nucl.}}$$

$$F_i = 4\pi R^2 \rho \left(4\pi R^2 \rho D_i \bullet \nabla_{\mathrm{M}} \mathcal{X} + v_i x_i\right), \ \nabla_{\mathrm{M}} \mathcal{X} = \left(\frac{\partial x_1}{\partial M}, \ldots, \frac{\partial x_{n_X}}{\partial M}\right)^{\mathrm{T}}$$

isotopes labelled by i with i=1, n_X

x_i : abundances per mole
$D_i = x_i B_i$ where B_i the i^{th} column of the diffusion matrix
v_i = advection velocity

NUMERICS

$$\frac{\partial x_i}{\partial t} = \frac{\partial F_i}{\partial M} + \left(\frac{\partial x_i}{\partial t}\right)_{\rm nucl.}$$

$$F_i = 4\pi R^2 \rho \left(4\pi R^2 \rho D_i \bullet \nabla_{\rm M}\mathcal{X} + v_i x_i\right), \ \nabla_{\rm M}\mathcal{X} = \left(\frac{\partial x_1}{\partial M}, \dots, \frac{\partial x_{n_{\rm X}}}{\partial M}\right)^{\rm T}$$

- The x_i are projected on to a finite set of piecewise polynomials, with discontinuous first derivative at the limits between radiative zone and convective zone.

- The piecewise polynomials, of degree m = 1, 2 or 3, are expressed with their B-spline basis $\{S_j\}$ of dimension n (~ number of grid points):

$$x_i(M) \simeq \sum_{j=1}^{n} x_{i,j} S_j(M) \text{ therefore } : \frac{{\rm d}x_i}{{\rm d}M} \simeq \sum_{j=1}^{n} x_{i,j} \frac{{\rm d}S_j}{{\rm d}M}$$

PRINCIPLES of THE GALERKIN METHOD

- defining the inner product

$$< f \bullet g > \equiv \int_{x_0}^{x_1} f g \, dx \Longrightarrow < df \bullet g > = [fg]_{x_0}^{x_1} - \int_{x_0}^{x_1} f dg \, dx = [fg]_{x_0}^{x_1} - < f \bullet dg >$$

- applied to the diffusion equations (with basis functions Sj)

$$< \frac{Dx_i}{Dt} \bullet S_j > = < \frac{\partial F_i}{\partial M} \bullet S_j > = [F_i S_j]_{M_0}^{M_1} - < F_i \bullet \frac{\partial S_j}{\partial M} >$$

- The *implicit* discretized diffusion equations become

$$< \left(\frac{x_i^{t+1} - x_i^t}{\Delta t}\right) \bullet S_j > + < F_i^{t+1} \bullet \frac{\partial S_j}{\partial M} > - [F_i^{t+1}]_{M_0}^{M_1} = 0$$

RESOLUTION of the SYSTEM

$$< \left(\frac{x_i^{t+1} - x_i^t}{\Delta t} \right) \bullet S_j > + < F_i^{t+1} \bullet \frac{\partial S_j}{\partial M} > - [F_i^{t+1}]_{M_0}^{M_1} = 0$$

n times n_X equations
for the n times n_X unknown coefficients : $x_{i,1}$ … $x_{i,n}$ with i = 1, …, n_X

the derivation operator affects the basis functions S_j and no longer the unknown functions x_i

the order of the differential equations is reduced by one unity.

$[F_i^{t+1}]_{M_0}^{M_1}$ is expressed with the boundaries conditions.

Efficient algorithms have been especially constructed for the calculations with B-splines.

the linear system to be solved is band-diagonal

MICROSCOPIC DIFFUSION in CESAM2k

Pressure, temperature, concentration gradients BUT no radiative accelerations

Michaud and Proffitt's formalism (1993)
hydrogen, helium diffusion
heavy elements as trace elts : diffusion results from collisions with protons
protons need to be present : valid on the main sequence only

Burger's formalism (1969)

With radiative accelerations

Work in progress in collaboration with G. Alecian

BURGERS'S FORMALISM

- Diffusion equation

$$\frac{\partial n_i}{\partial t} = \frac{1}{x^2}\frac{\partial}{\partial x}(x^2 n_i w_i), \;\; w_i = \sum_{j=1}^{nx} b_{i,j}\frac{\partial x_j}{\partial x} + v_i$$

n_i : density of isotope i

- Burgers's equations : no conduction current, no magnetic field

$$\frac{dP_i}{dR} - \frac{\rho_i}{\rho}\frac{dP}{dR} - n_i \bar{z}_i eE = \sum_j K_{i,j}(w_j - w_i) + \sum_j K_{i,j} z_{i,j}\frac{m_j r_i - m_i r_j}{m_i + m_j}$$
$$\frac{5}{2} n_i k \frac{dT}{dR} = -\frac{5}{2}\sum_j K_{i,j} z_{i,j}\frac{m_j(w_j - w_i)}{m_i + m_j} - \frac{2}{5} K_{ii} z''_{ii} r_i$$
$$-r_i \sum_{j\neq i} K_{i,j}\frac{3m_i^2 + m_j^2 z'_{i,j} + \frac{4}{5} m_i m_j z''_{i,j}}{(m_i+m_j)^2} + \sum_{j\neq i} K_{i,j}\frac{m_i m_j (3 + z'_{i,j} - \frac{4}{5} z''_{i,j})}{(m_i+m_j)^2} r_j$$

BURGERS'S FORMALISM

- Burgers's equations

$$\frac{dP_i}{dR} - \frac{\rho_i}{\rho}\frac{dP}{dR} - n_i \bar{z}_i eE = \sum_j K_{i,j}(w_j - w_i) + \sum_j K_{i,j} z_{i,j}\frac{m_j r_i - m_i r_j}{m_i + m_j}$$
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collisions integrals from Paquette et al. (1986) K_{ij} z_{ij} z'_{ij} z''_{ij}

mean charge from Saha equation $\bar{Z}_i$

BURGERS'S EQUATIONS

$$\frac{dP_i}{dR} - \frac{\rho_i}{\rho}\frac{dP}{dR} - n_i \bar{z}_i eE = \sum_j K_{i,j}(w_j - w_i) + \sum_j K_{i,j} z_{i,j} \frac{m_j r_i - m_i r_j}{m_i + m_j}$$

$$\frac{5}{2} n_i k \frac{dT}{dR} = -\frac{5}{2} \sum_j K_{i,j} z_{i,j} \frac{m_j(w_j - w_i)}{m_i + m_j} - \frac{2}{5} K_{ii} z''_{ii} r_i$$

$$-r_i \sum_{j \neq i} K_{i,j} \frac{3m_i^2 + m_j^2 z'_{i,j} + \frac{4}{5} m_i m_j z''_{i,j}}{(m_i + m_j)^2} + \sum_{j \neq i} K_{i,j} \frac{m_i m_j (3 + z'_{i,j} - \frac{4}{5} z''_{i,j})}{(m_i + m_j)^2} r_j$$

- With dynamical conservation of mass and charge

$$\sum_{i=1}^{n_X} x_i \nu_i w_i = 0, \quad \sum_{i=1}^{n_X+1} \bar{z}_i x_i w_i = 0$$

- The equations become a linear system

$$A\omega = \gamma + G\,D_R, \ D_R = \left(\frac{\partial x_1}{\partial R}, \ldots, \frac{\partial x_{n_X}}{\partial R}, 0, \ldots, 0\right)^T$$

SOLUTIONS of BURGERS'S EQUATIONS

- linear system

$$A\omega = \gamma + G\,D_R, \ D_R = \left(\frac{\partial x_1}{\partial R}, \ldots, \frac{\partial x_{n_X}}{\partial R}, 0, \ldots, 0\right)^T$$

- with solutions

$$\omega = V + B\,D_R, \ V = A^{-1}\gamma, \ B = A^{-1}G$$

$i,j = 1, \ldots, n_x$,
$b_{i,j}$ and v_i, are coefficients of B and V

CONTROL of GRAVITATIONNAL SETTLING

High masses : too large gravitational settling of helium and heavy elements

CESAM : OPTIONNAL
control by the turbulence resulting from the radiative viscosity

radiative viscosity due to the energy exchanges between thermal collisions leading to excitation and ionization of atoms and ions (Mihalas & Weibel-Mihalas, 1984)

$$d_\nu = Re_\nu \frac{4}{15} \frac{aT^4}{c\kappa\rho^2}$$

$Re_\nu \sim 1$ (Morel & Thévenin, 2002).

The physical origin of this coefficient and simple formalism, have been much questioned by Alecian & Michaud (2005).