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Modelling of Turbulent Composition Flux in Stars

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ABSTRACT
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Key words: turbulence – mixing – nuclear burning – stellar evolution

1 INTRODUCTION

Turbulent composition flux is the key property which represent transport of chemical elements in stars. To get it right is essential, because in reactive flows like core convection in stars, mixing controls rate of nuclear reactions, and eventually stellar yields.

In this paper, we study turbulent composition flux in a 3D cartesian box (non-reactive) turbulence with 2 fluids, where fluid1 is located in the unstable half at bottom and the fluid2 in stable half at top (Fig.1) and based on our results judge accuracy of known modelling approaches to this problem.

We focus on four approaches, which are most viable for modelling of turbulent flux for problems in stellar evolution, namely (i) diffusion approximation (ii) composition flux equation model (iii) algebraic models (iv) integral models and (v) GANS models based on artificial intelligence.

Turbulent composition flux is

$$f_i = \overline{\rho}\widetilde{X_i'' u_r''} \quad (1)$$

2 DIFFUSION MODEL

Diffusion approximation is

$$f_i = -\,D\ \rho\ \partial_r \widetilde{X}_i \quad (2)$$

Following Eggleton (1973), common approximations to composition flux in calculations of stellar evolution typically utilize a diffusion operator $\mathcal{D} \equiv -D\partial_r$ applied to a background mass fraction profile of an element whose transport we want to simulate. The D is the diffusivity and defined in most cases as

$$D = \frac{1}{3}\ u_{MLT}\ (\alpha H_P) \quad (3)$$

where u_{MLT} is the mixing length velocity (Eq.4), α is the mixing length parameter and H_p is the pressure scale height (e.g., Heger et al. 2000; Paxton et al. 2011). Arnett et al. (2015) suggest that this approximation is inadequate, based upon an investigation focusing on the turbulent velocity field; here we extend this investigation to composition.

$$u_{MLT} = \frac{f_h}{\alpha_E \rho c_P (T')_{rms}} \quad (4)$$

The fluid1 and fluid2 flux calculated by this diffusion approximation is badly in error (Fig.3, Fig.4).

Within the convection zone, where composition gradients are shallow but velocities are large, again the diffusion approximation does not give a good estimate of the turbulent fluxes (but is at least correct to an order of magnitude). The inaccuracy of the diffusive mixing approximation may be quantified by comparing these heuristic diffusivities (Eq. 3) to the the effective diffusivity D_{eff}, which *would be needed to reproduce the correct flux,*

$$D_{eff} = -f_i/(\overline{\rho}\partial_r \widetilde{X}_i). \quad (5)$$

There is an added complication, which is shown in Fig. 3 due to local maximum/minimum in fluid1/fluid2 mass fraction X around $r \sim 5.8 \times 10^8$ cm. Applying the diffusion approximation to the turbulent flux there gives an even more peculiar result, due to this non-monotonic profile of fluid1 and fluid2 mass fraction (Fig. 3). This requires a discontinuous behavior of the effective diffusivity (Fig.3) to reproduce the correct flux. *The actual flux in the 3D simulation is well-behaved;*

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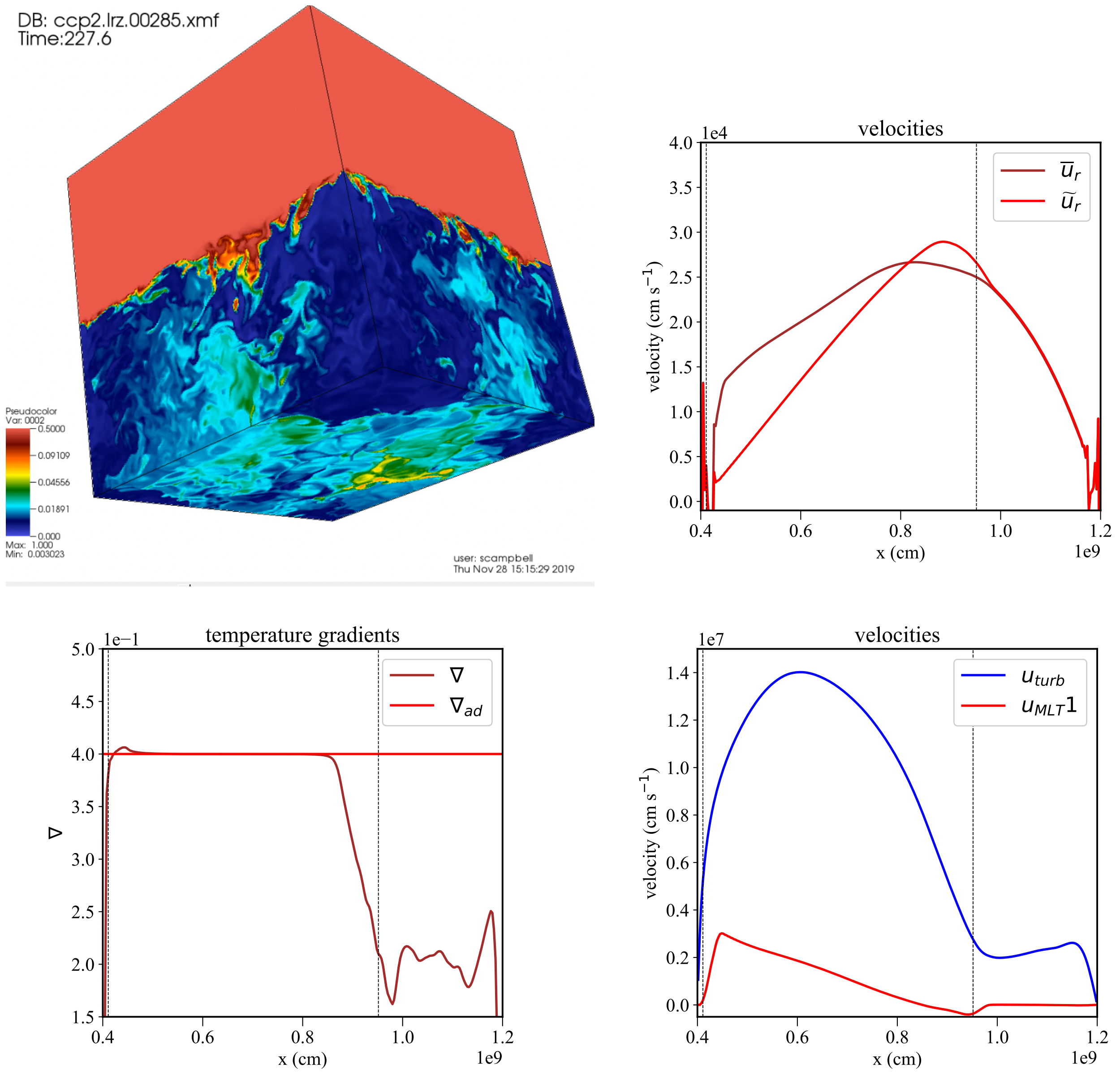

Figure 1. Top-Left: 3D visualization of the model. Top-Right: Mean background velocities of the 3D model. Bottom-Left: Temperature gradient in the 3D model. Bottom-Right: Velocities. alphae for uMLT is here 0.2 - quite small, if I remember correctly, Arnett 2019 say 0.5, Meakin et al, 0.7

3 COMPOSITION FLUX EQUATION MODEL

$$\partial_t \widetilde{X}_i = + \dot{X}_i^{nuc} - (1/\overline{\rho})\nabla_x f_i - \widetilde{u}_x \partial_x \widetilde{X}_i \qquad (6)$$

$$\overline{\rho}\partial_t(f_i/\overline{\rho}) = -\nabla_x f_i^r - f_i \partial_x \widetilde{u}_x - \widetilde{R}_{xx}\partial_x \widetilde{X}_i - \overline{X_i''\partial_x P} \qquad (7)$$

$$+\overline{u_x''\rho\dot{X}_i^{\rm nuc}} - \overline{\rho}\widetilde{u}_x\partial_x f_i/\overline{\rho} \qquad (8)$$

$$\text{where} \qquad (9)$$

$$f_i^r = -D\partial_x f_i \qquad (10)$$

$$\widetilde{R}_{rr} = +\mathrm{model}_{rxx} \qquad (11)$$

$$\overline{X_i''\partial_x P} = +\mathrm{model}_{xgrp} \qquad (12)$$

$$\overline{u_x''\rho\dot{X}_i^{\rm nuc}} = +\mathrm{model}_{udxn} \qquad (13)$$

4 ALGEBRAIC MODEL

Rogers1989

$$\overline{\rho}\partial_t(f_i/\overline{\rho}) = -f_i\partial_x\widetilde{u}_x - \widetilde{R}_{xx}\partial_x\widetilde{X}_i + \psi_i \qquad (14)$$

$$\text{where } \psi_i = -\nabla_x f_i^x - \overline{X_i''\partial_x P} + \overline{u_x''\rho\dot{X}_i^{\rm nuc}} + -\overline{\rho}\widetilde{u}_x\partial_x f_i/\overline{\rho}$$

Let us assume the flux is quasi-static $\overline{\rho}\partial_t(f_i/\overline{\rho}) = 0$ and $\psi_i = +(C_D/\tau)f_i$. We get

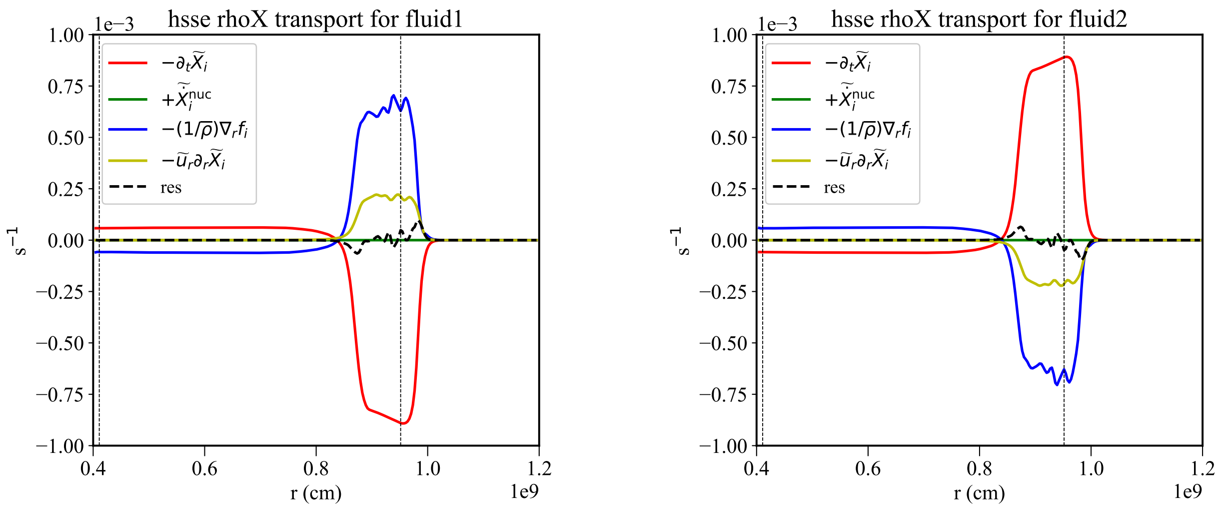

Figure 2. Hydrodynamic stellar structure composition equations for fluid1 and fluid2.

$$
\begin{aligned}
0 =& - f_i \partial_x \widetilde{u}_x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i + \psi_i \quad \text{quasi-static flux} && (15)\\
0 =& - f_i \partial_x \widetilde{u}_x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i + (C_D/\tau) f_i && (16)\\
\mathcal{O}_x f_i =& - \widetilde{R}_{rr} \partial_x \widetilde{X}_i \quad \text{where} \quad \mathcal{O}_x = C_D/\tau - \partial_x \widetilde{u}_x && (17)\\
f_i =& - \mathcal{O}_x^{-1} \widetilde{R}_{rr} \partial_x \widetilde{X}_i \quad \text{algebraic model for } f_i && (18)\\
\text{where}& && (19)\\
f_i =& + \overline{\rho} \widetilde{X_i'' u_x''} \quad \text{composition flux for element } i && (20)\\
f_i^x =& + \overline{\rho} \widetilde{X_i'' u_x'' u_x''} \quad \text{flux of composition flux} && (21)\\
\widetilde{R}_{xx} =& + \overline{\rho} \widetilde{u_x'' u_x''} \quad \text{Reynolds stress} && (22)
\end{aligned}
$$

5 INTEGRAL MODELS

Based on the mean fields in fluid1 and fluid2 flux equations (Fig.5), we can do similar algebraic manipulations as in previous section, but arrive at integral model instead.

$$
\begin{aligned}
0 =& - \nabla_x f_i^x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i - \overline{X'' \rho g_x} && (23)\\
0 =& - \nabla_x f_i^x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i - \overline{(X - \widetilde{X}) \rho g_x} && (24)\\
0 =& - \nabla_x f_i^x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i - \overline{\rho X} \overline{g}_x + \widetilde{X} \overline{\rho g}_x && (25)\\
0 =& - \nabla_x f_i^x - \widetilde{R}_{xx} \partial_x \widetilde{X}_i && (26)\\
f_i^x =& \int R_{xx} \partial_x \widetilde{X} dx && (27)\\
f_i =& \int \int R_{xx} \partial_x \widetilde{X} dx^2 \quad \text{where } f_i^x \sim c_D \partial_x f_i && (28)
\end{aligned}
$$

6 GANS - CAN AI HELP

try to find out how to use AI to give us right model

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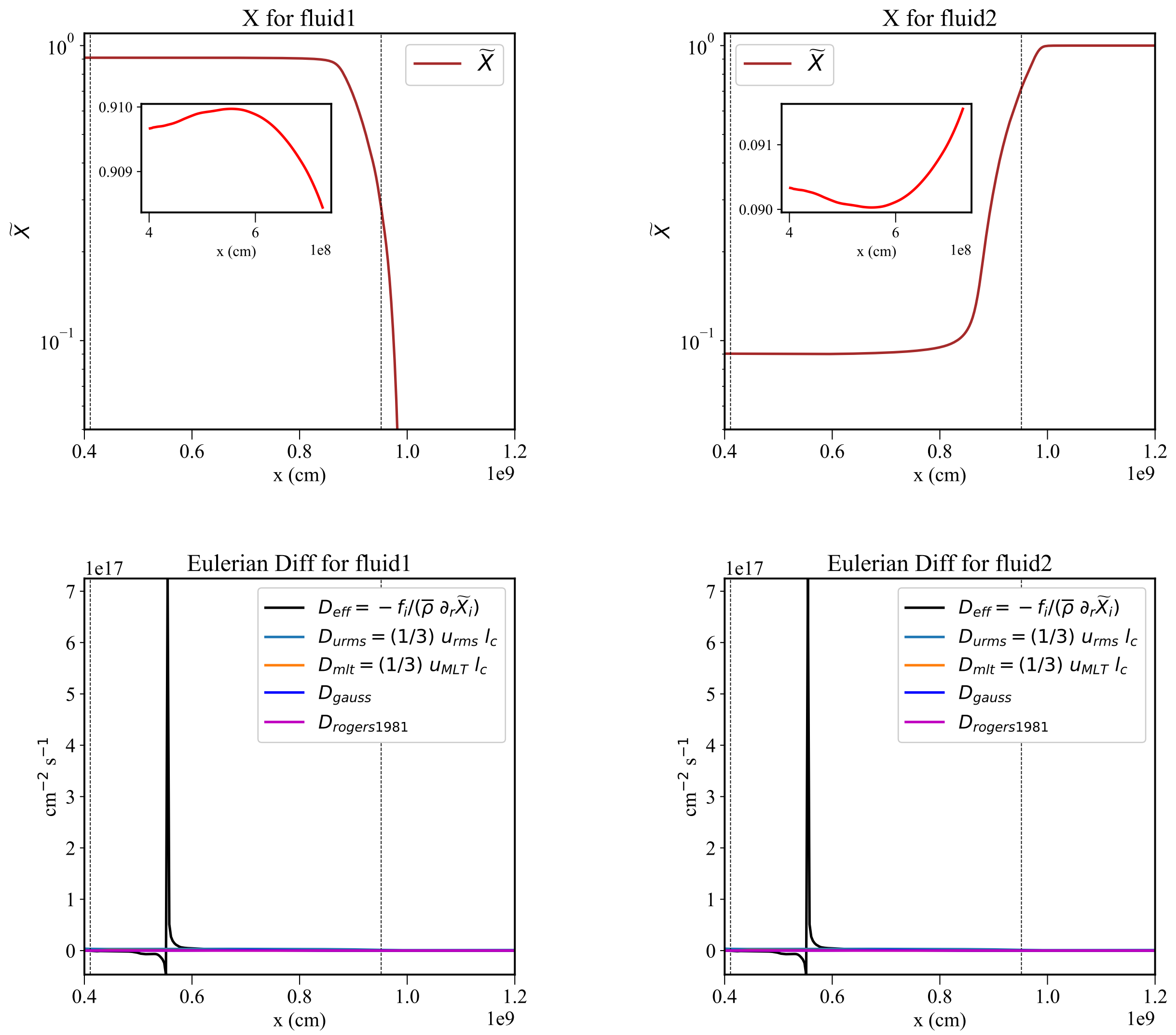

Figure 3. Top: Mass fraction of fluid1 and fluid2. Bottom: Diffusivities for fluid1 and fluid2.

Table 1. Definitions:

$$
\begin{array}{ll}
\rho \ \ \text{density} & g_x \ \ \text{radial gravitational acceleration} \\
m = \rho V = \rho \frac{4}{3}\pi r^3 \ \ \text{mass} & M = \int \rho(r) dV = \int \rho(r) 4\pi r^2 dr \ \ \text{integrated mass} \\
T \ \ \text{temperature} & \mathcal{S} = \rho\epsilon_{\rm nuc}(q) \ \ \text{nuclear energy production (cooling function)} \\
P \ \ \text{pressure} & \tau_{ij} = 2\mu S_{ij} \ \ \text{viscous stress tensor} \ \ (\mu \ \ \text{kinematic viscosity}) \\
u_x, u_\theta, u_\phi \ \ \text{velocity components} & S_{ij} = (1/2)(\partial_i u_j + \partial_j u_i) \ \ \text{strain rate} \\
\mathbf{u} = u(u_x, u_\theta, u_\phi) \ \ \text{velocity} & \widetilde{R}_{ij} = \overline{\rho}\widetilde{u''_i u''_j} \ \ \text{Reynolds stress tensor} \\
f_i = \overline{\rho}\widetilde{X''_i u''_x} &
\end{array}
\tag{29}
$$

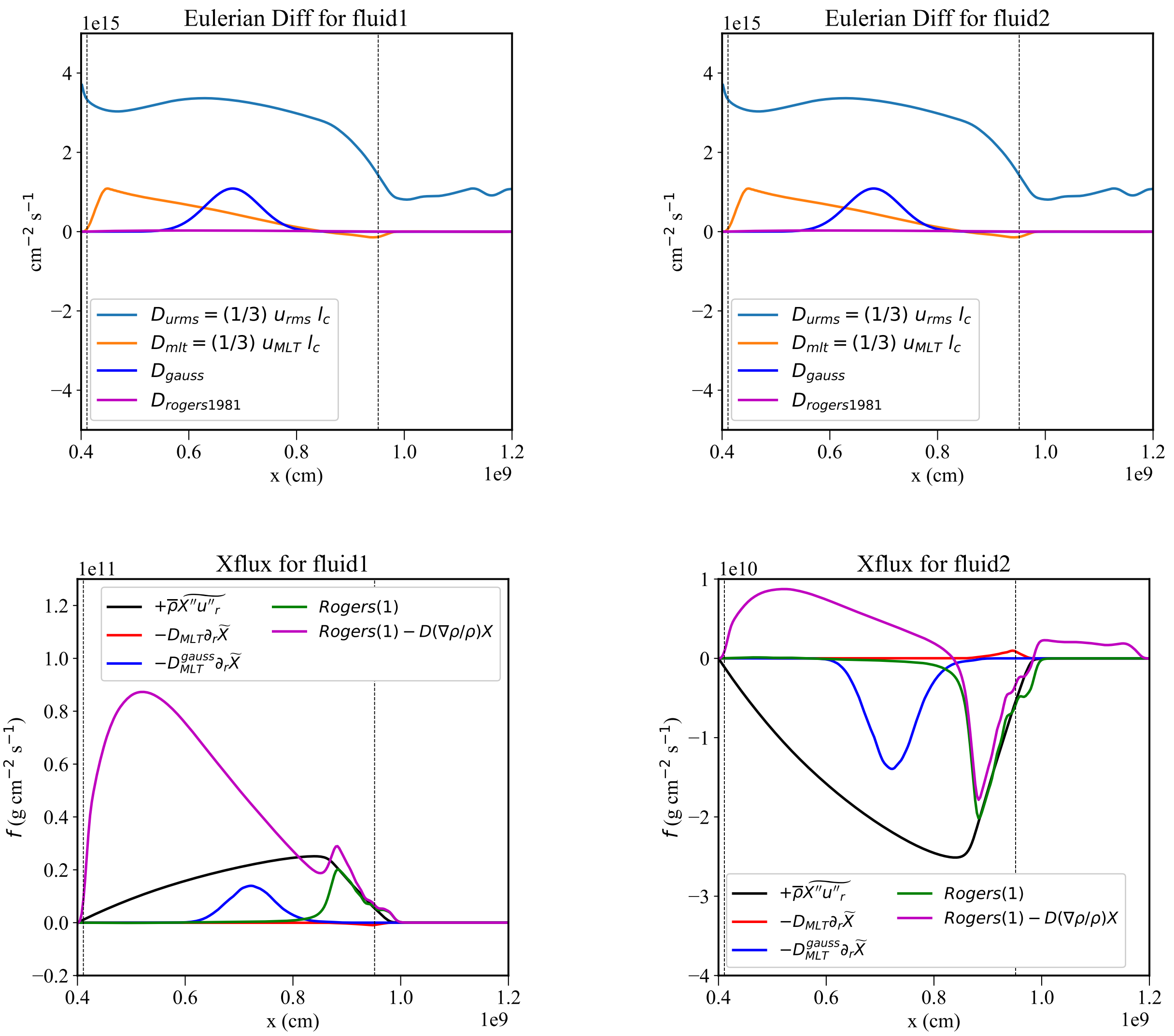

Figure 4. Top: Diffusivities for fluid1 and fluid2. Bottom: Turbulent composition flux and diffusion models for fluid1 and fluid2.

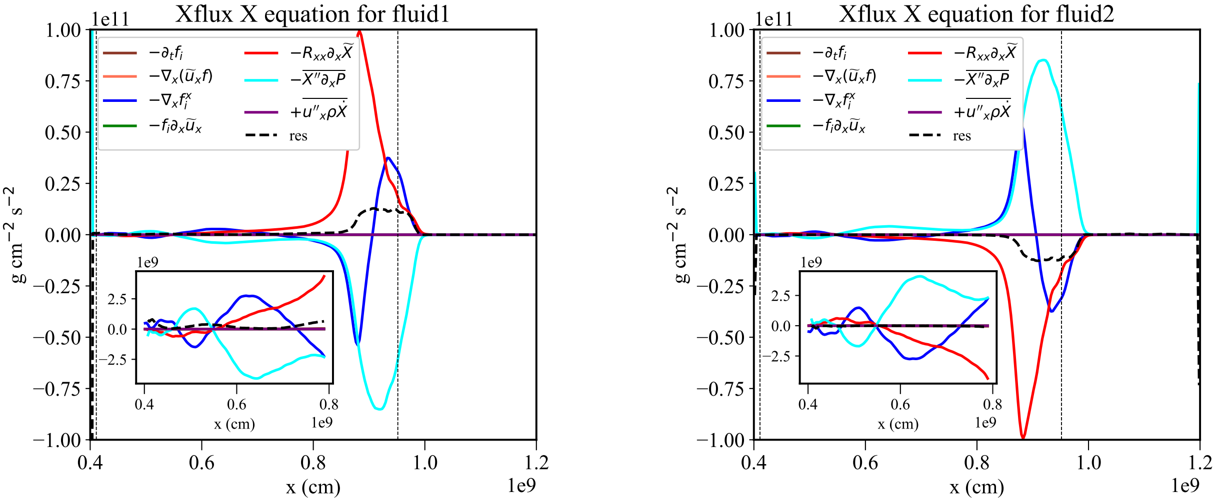

Figure 5. Turbulent composition flux equations for fluid1 and fluid2.

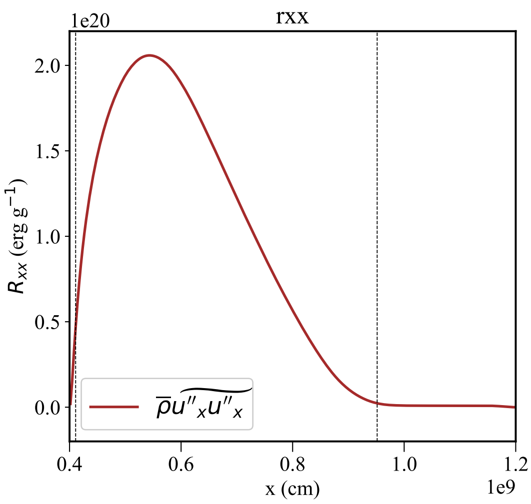

Figure 6. Profile for Reynolds stress.

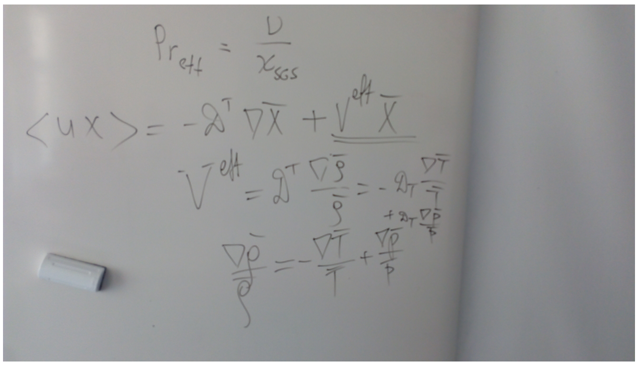

Figure 7. Turbulent-thermal diffusion model - notes from NORDITA workshop in Stockholm.