Rogers et al. [1989] to ransX mapping with focus on composition mass fraction X_α and development of turbulent scalar flux models for stars

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This is an attempt to apply methods by Rogers et al. [1989], who derive models for turbulent passive (no feedback on flow's velocity field) scalar flux in incompressible ($\nabla \cdot u' = 0$) homogeneous ($\rho = const.$, mean velocity and scalar field unaffected by turbulence, no spatial gradients in scalar flux) simple shear flow to compressible inhomogeneous shear flows with active scalars and gravity in stars. Einstein summation convention used here. Our passive/active scalars will be mass fractions of chemical elements X_α subjected to nuc burning $\dot{X}_\alpha^{nuc}$, where $\sum_\alpha X_\alpha = 1$.

1 Governing equations for homogeneous and incompressible flow without gravity and its passive scalar turbulent flux

[Rogers et al., 1989]	**[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]**

governing Equations

[Rogers et al., 1989]	ransX
$U_{i,i} = 0$	$\partial_i u_i = 0$
$\partial_t U_i + U_j U_{i,j} + (1/\rho) P_{,i} = \nu \ U_{i,jj}$	$\partial_t u_i + u_j \partial_j u_i + (1/\rho)\partial_i P = +\nabla_j \tau_{ij}$
$\partial_t T + U_j T_{,j} = \gamma \ T_{,jj} + \Sigma$	$\partial_t X_\alpha + u_j \partial_j X_\alpha = \gamma \underbrace{\nabla_j \partial_j X_\alpha}_{\text{diffusion, divergence of gradient}} + \dot{X}_\alpha^{nuc}$

$$meanField\ decomposition$$

$$u_i = \overline{U}_i + u'_i \quad P = \overline{P} + p' \quad T = \overline{T} + \theta$$

$$u_i = \overline{u}_i + u'_i \quad P = \overline{P} + P' \quad X = \overline{X} + X'$$

$$meanField\ equations$$

$$\overline{U}_{i,i} = 0$$

$$\partial \overline{U}_i + \overline{U}_j \overline{U}_{i,j} + (\overline{u_i u_j})_{,j} + (1/\rho)\overline{P}_{,i} = \nu \ \overline{U}_{i,jj}$$

$$\partial_t \overline{T} + \overline{U}_j \overline{T}_{,j} + (\overline{\theta u_j})_{,j} = \gamma \ \overline{T}_{,jj} + \Sigma$$

$$\partial_t \overline{\theta u_i} = -\overline{u_i u_j}\overline{T}_{,j} - \overline{\theta u_j} \ \overline{U}_{i,j} + (1/\rho) \ \overline{p\theta_{,i}} - (\nu + \gamma) \ \overline{u_{i,j}} \ \overline{\theta_{,j}}$$
$$- \left(\overline{\theta u_i} \ \overline{U}_j + \overline{\theta u_i u_j} + (1/\rho) \ \overline{p\theta}\delta_{ij} - \nu \ \overline{\theta u_{i,j}} - \gamma \ \overline{u_i} \ \overline{\theta_{,j}}\right)_{,j}$$

$$\partial_i \overline{u}_i = 0$$

$$\partial_t \overline{u}_i + \overline{u}_j \partial_j \overline{u}_i + \underbrace{\nabla_j \overline{u'_i u'_j} - \cancelto{0 \ incompressible}{\overline{u'_i \nabla_j u'_j}}}_{\overline{u'_j \partial_j u'_i}} + (1/\rho)\partial_i \overline{P} - \overline{g}_i = \overline{\nabla_j \tau_{ij}}$$

$$\partial_t \overline{X}_\alpha + \overline{u}_j \partial_j \overline{X}_\alpha + \underbrace{\nabla_j \overline{X'_\alpha u'_j} - \cancelto{0}{\overline{X'_\alpha \nabla_j u'_j}}}_{\overline{u'_j \partial_j X'}} = \gamma \ \overline{\nabla_j \partial_j \overline{X}_\alpha} + \overline{\dot{X}^{nuc}_\alpha}$$

$$\partial_t \overline{X'_\alpha u'_i} = -\overline{u'_i u'_j}\partial_j \overline{X} - \overline{X'_\alpha u'_j}\partial_j \overline{u}_i - (1/\rho)\overline{X' \partial_i P'} + \overline{X' \nabla_j \tau_{ij}}$$
$$- \left(\nabla_j \overline{X' u'_j u'_i}\right) - \overline{X' u'_i d'} - \overline{u}_i \partial_i \overline{X' u'_i}$$

1.1 Governing equations for assumed turbulent shear flow in Figure 1

[Rogers et al., 1989]

$$\overline{U}_{1,1} = 0$$
$$\partial_t \overline{U}_1 + (1/\rho)\overline{P}_{,1} = 0 \quad \overline{P}_{,2} = 0 \quad \overline{P}_{,3} = 0$$
$$\partial_t \overline{T} + (S \ x_2) \ \overline{T}_{,1} = \Sigma$$

[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]

$$\partial_x u_x = 0$$
$$\partial_t \overline{u}_x + (1/\rho)\partial_x \overline{P} = 0 \quad \partial_y \overline{P} = 0 \quad \partial_z \overline{P} = 0$$
$$\partial_t \overline{X}_\alpha + (S \ y) \ \partial_x \overline{X}_\alpha = +\overline{\dot{X}^{nuc}_\alpha}$$

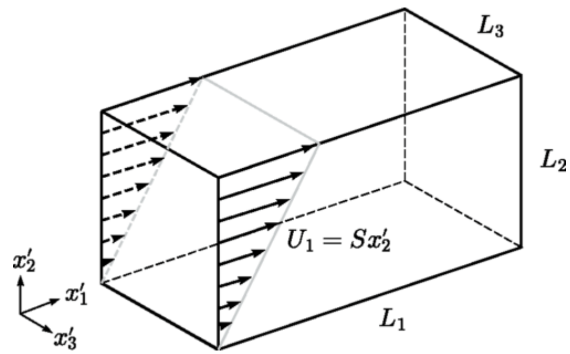


Figure 1: Schematic representation of homogeneous ($\rho = const.$) turbulent shear ow conguration, with $\overline{U}_1(x_2) = S\ x_2, \overline{U}_2 = 0, \overline{U}_3 = 0$ as the mean velocities, $S = \partial_2 \overline{U}_1$ the imposed uniform mean shear and (L_1, L_2, L_3) representing the domain size.

Some required definitions from [Rogers et al., 1989]:

$$
\begin{aligned}
S_\theta &= \partial_i \overline{T} \ \text{ mean scalar gradient magnitude} \\
\theta' &= \overline{\theta^2}^{1/2} \ \text{ rms of scalar fluctuation } \theta \\
\sigma^{\theta}_{diss} &= 2\ \gamma\ \partial_j \overline{X' \partial_j X'} = 2\chi \ \text{ dissipation of scalar fluctuations} \\
\gamma & \ \text{ kinematic/molecular diffusivity of passive scalars}
\end{aligned} \tag{1}
$$

$$
\begin{aligned}
S &= \partial_2 \overline{U}_1 \ \text{ mean shear rate} \\
q^2 &= \overline{u_i' u_i'} \ \text{ Reynolds stress tensor} \\
\epsilon &= \nu\ \overline{\partial_j u_i' \partial_j u_i'} \ \text{ dissipation of TKE} \\
\nu & \quad \text{kinematic viscosity}
\end{aligned} \tag{2}
$$

The quantities $S_\theta, \theta', \chi, \gamma$ are analogous to the quantities S, q, ϵ, ν characterizing the behaviour of the velocity field. From these scales a lengthscale θ'/S_θ and a timescale $(\theta')^2/\chi$ can be formed. The ratios of the analogous scales of the velocity field to these two scales yield two dimensionless parameters:

$$
B = \frac{(q/S)}{(\theta'/S_\theta)} \sim const_1 \quad R = \frac{(q^2/\epsilon)}{((\theta')^2/\chi)} \sim const_2 \ \text{ constants depend on Prandtl number and orientation of mean scalar gradient} \tag{3}
$$

- B represents the relative strenght of the fluctuating velocity field compared to the fluctuating scalar field (for the simple shear flow $B \sim 0.5 - 1.1$)
- R represents the ratio of the hydrodynamic turbulence timescale to the scalar turbulence timescale (for the simple shear flow $R \sim 2$)

1.2 Turbulent scalar flux models derivation

Because the scalar flux is based on the behaviour of a passive scalar that does not affect the velocity field, it is reasonalbe to expect that it would be possible to model this quantity based solely on characteristics of the velocity field, the imposed uniform scalar gradient and the Prandtl number.

The simplest gradient transport model is:

[Rogers et al., 1989]	**[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]**
$\overline{\theta u_i} = -\gamma_T \ \partial_i \overline{T}$	$\overline{X' u'_i} = -\gamma_T \ \partial_i \overline{X}_\alpha$

γ_T is turbulent eddy diffusivity. This works only if the scalar flux is aligned with the mean scalar gradient. But, **the scalar flux in homogeneous turbulent shear flow is not, in general, aligned with the mean scalar gradient!** Additionally, the magnitude of the flux component down the gradient varies substantially, depending on the direction of the imposed mean scalar gradient.

Because the simple gradient transport model cannot represent the behaviour of the scalar flux using a scalar turbulent eddy diffusivity γ_T, it becomes necessary to implement a tensor eddy diffusivity as suggested by Batchelor (1949). This yields:

[Rogers et al., 1989]	**[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]**	
$\overline{\theta u_i} = -D_{ij} \ \partial_j \overline{T}$	$\overline{X' u'_i} = -D_{ij} \ \partial_j \overline{X}_\alpha$	(4)

where D_{ij} is the turbulent eddy diffusivity tensor (gradient of vector field). Because the flux vector is not aligned with the mean scalar gradient, D_{ij} is not a diagonal tensor. For the assumed coordinate system (Fig.1), flow symetry implies $D_{13} = D_{23} = D_{31} = D_{32} = 0$.

The governing equation for the turbulent scalar flux in homogeneous flows is[1]:

[Rogers et al., 1989]

$$\partial_t \overline{\theta u_i} = -\overline{u_i u_j}\,\overline{T}_{,j} - \overline{\theta u_j}\ \overline{U}_{i,j} + \psi_i$$
$$\psi_i = +(1/\rho)\ \overline{p\theta_{,i}} - (\nu + \gamma)\ \overline{u_{i,j}}\ \overline{\theta_{,j}}$$

[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]

$$\partial_t \overline{X'_\alpha u'_i} = -\overline{u'_i u'_j}\partial_j \overline{X} - \overline{X'_\alpha u'_j}\partial_j \overline{u}_i + \psi_i$$
$$\psi_i = +(1/\rho)\overline{P'\partial_i X'_\alpha} + \overline{X'\nabla_j \tau_{ij}}$$

One of the key arguments of Rogers et al. [1989] is that correlation coefficient $\overline{\theta u_i}/\theta' q$ does appear to reach a constant value when the flow becomes developed, implying that $\partial_t(\overline{\theta u_i}/\theta' q)$. Differentiation together with the governing equations for turbulent kinetic energy and the scalar fluctuation intensity then yields [2]

$$\frac{\partial \overline{\theta u'_i}}{\partial t} \sim \frac{\overline{\theta u_i}}{q^2}(\mathcal{P} - \epsilon) + \frac{\overline{\theta u_i}}{\overline{\theta}^2}(\mathcal{P}_\theta - \chi) = \text{scalar} \times \overline{\theta u_i} \tag{5}$$

where $\mathcal{P} = -\overline{u_1 u_2}S$ and $\mathcal{P}_\theta = -\overline{\theta u_j}\overline{T}_{,j}$ denote the production rates of $(1/2)q^2$ and $(1/2)\overline{\theta}^2$, respectively. This indicates that the change of θu_i is exactly aligned with θu_i itself. The dissipation term $-(\nu + \gamma)\ \overline{u_{i,j}}$ is typically small for high Reynolds numbers. It thus seems reasonable that both ϕ_i and the time change of the scalar flux can be replaced by a multiple of the scalar flux vector, yielding

[Rogers et al., 1989]

$$0 = -\overline{u_i u_j}\,\overline{T}_{,j} - \overline{\theta u_j}\ \overline{U}_{i,j} - C_D \frac{1}{\tau}\overline{\theta u_i}$$
$$\mathcal{O}_{ij}\overline{\theta u_j} = -\overline{u_i u_j}\,\overline{T}_{,j} \quad \text{where} \quad \mathcal{O}_{ij} = (C_D/\tau)\delta_{ij} + \overline{U}_{i,j}$$

[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]

$$0 = -\overline{u'_i u'_j}\partial_j \overline{X}_\alpha - \overline{X'_\alpha u'_j}\partial_j \overline{u}_i - C_D \frac{1}{\tau}\overline{X'_\alpha u'_i}$$
$$\mathcal{O}_{ij}\overline{\theta u_j} = -\overline{u'_i u'_j}\partial_j \overline{X}_\alpha \quad \text{where} \quad \mathcal{O}_{ij} = (C_D/\tau)\delta_{ij} + \partial_j \overline{u}_i$$

where C_D dimensionless coefficient and τ is an appropriate timescale[3]. This equation implies that the sum of the two scaler flux production

[1]some terms derived in Section 1 must be zero, where did they go and why, is it due to the assumed problem definition as shown in Fig.1? $-\left(\overline{\theta u_i}\ \overline{U}_j + \overline{\theta u_i u_j} + (1/\rho)\ \overline{p\theta}\delta_{ij} - \nu\ \overline{\theta u_{i,j}} - \gamma\ \overline{u_i}\ \overline{\theta_{,j}}\right)_{,j} = 0$ [Rogers et al., 1989] $-\left(\nabla_j \overline{X' u'_j u'_i} + (1/\rho)\partial_j \overline{P' X'_\alpha}\right) - \overline{X' u'_i d'} - \overline{u}_i \partial_i \overline{X' u'_i} = 0\ (ransX)$. Yes, [Rogers et al., 1989], page 79 - The term is zero in homogeneous flows. But it is just a statement there without any arguments in favor.

[2]this is not obvious to me, where did they get the scalar fluctuation intensity equation from? authors never mention it.

[3]Perhaps dissipation timescale for TKE or scalar variance?

terms is aligned with the scalar flux vector, an easier assumption to check in practice that the alilgnement of the modelled terms witht the flux vector. **The governing equation has now been reduced to an algebraic equation for θu_i and can be solved.**[4]

$$
\begin{aligned}
\overline{\theta u_i} &= -\ D^M_{ij}\ \partial_j \overline{T} = -O^{-1}_{in} \overline{u_n u_j}\ \partial_j \overline{T} = -(1/2)(\mathcal{O}^{-1} \epsilon_{pki} \epsilon_{lmn} \mathcal{O}_{lp} \mathcal{O}_{mk} \overline{u_n u_j})\ \partial_j \overline{T} \\
\overline{X'_\alpha u'_i} &= -\ D^M_{ij}\ \partial_j \overline{X} = -O^{-1}_{in} \overline{u'_n u'_j}\ \partial_j \overline{X} = -(1/2)(\mathcal{O}^{-1} \epsilon_{pki} \epsilon_{lmn} \mathcal{O}_{lp} \mathcal{O}_{mk} \overline{u'_n u'_j})\ \partial_j \overline{X} \quad \text{ransX equivalent}
\end{aligned}
\tag{6}
$$

On component basis for the shear flow:

[Rogers et al., 1989]	**[ransX nomenclature equivalent with focus on $\mathbf{X}_\alpha$]**
$D^M_{11} = +(\tau/C_D)\ \overline{u_1 u_1} - S\ \tau\ (\tau/C^2_D)\ \overline{u_1 u_2}$	$D^M_{11} = +(\tau/C_D)\ \overline{u'_1 u'_1} - S\ \tau\ (\tau/C^2_D)\ \overline{u'_1 u'_2}$
$D^M_{12} = +(\tau/C_D)\ \overline{u_1 u_2} - S\ \tau\ (\tau/C^2_D)\ \overline{u_2 u_2}$	$D^M_{12} = +(\tau/C_D)\ \overline{u'_1 u'_2} - S\ \tau\ (\tau/C^2_D)\ \overline{u'_2 u'_2}$
$D^M_{21} = +(\tau/C_D)\ \overline{u_1 u_2}$	$D^M_{21} = +(\tau/C_D)\ \overline{u'_1 u'_2}$
$D^M_{22} = +(\tau/C_D)\ \overline{u_2 u_2}$	$D^M_{22} = +(\tau/C_D)\ \overline{u'_2 u'_2}$
$D^M_{33} = +(\tau/C_D)\ \overline{u_3 u_3}$	$D^M_{33} = +(\tau/C_D)\ \overline{u'_3 u'_3}$

Turbulent convection in stars is not a shear flow, it is neither homogeneous and incompressible, but let's assume it is now and either a shear between upflows and downflows or upflows/downflows shearing against convection boundaries. We'll see in th next subsection, that **for radial turbulent flux this model is not working.** It either understimate the flux in the convection zone or overestimate at convection boundaries.

1.2.1 Shear between upflows and downflows

Geometry specification: $(1 = r, 2 = \theta, 3 = \phi)$, mean shear rates $S_{r\theta} = +\overline{\partial_\theta u_r}$, $S_{r\phi} = +\overline{\partial_\theta u_r}$, $\tau = \widetilde{k}/\sigma_k$, $C_D = 100$

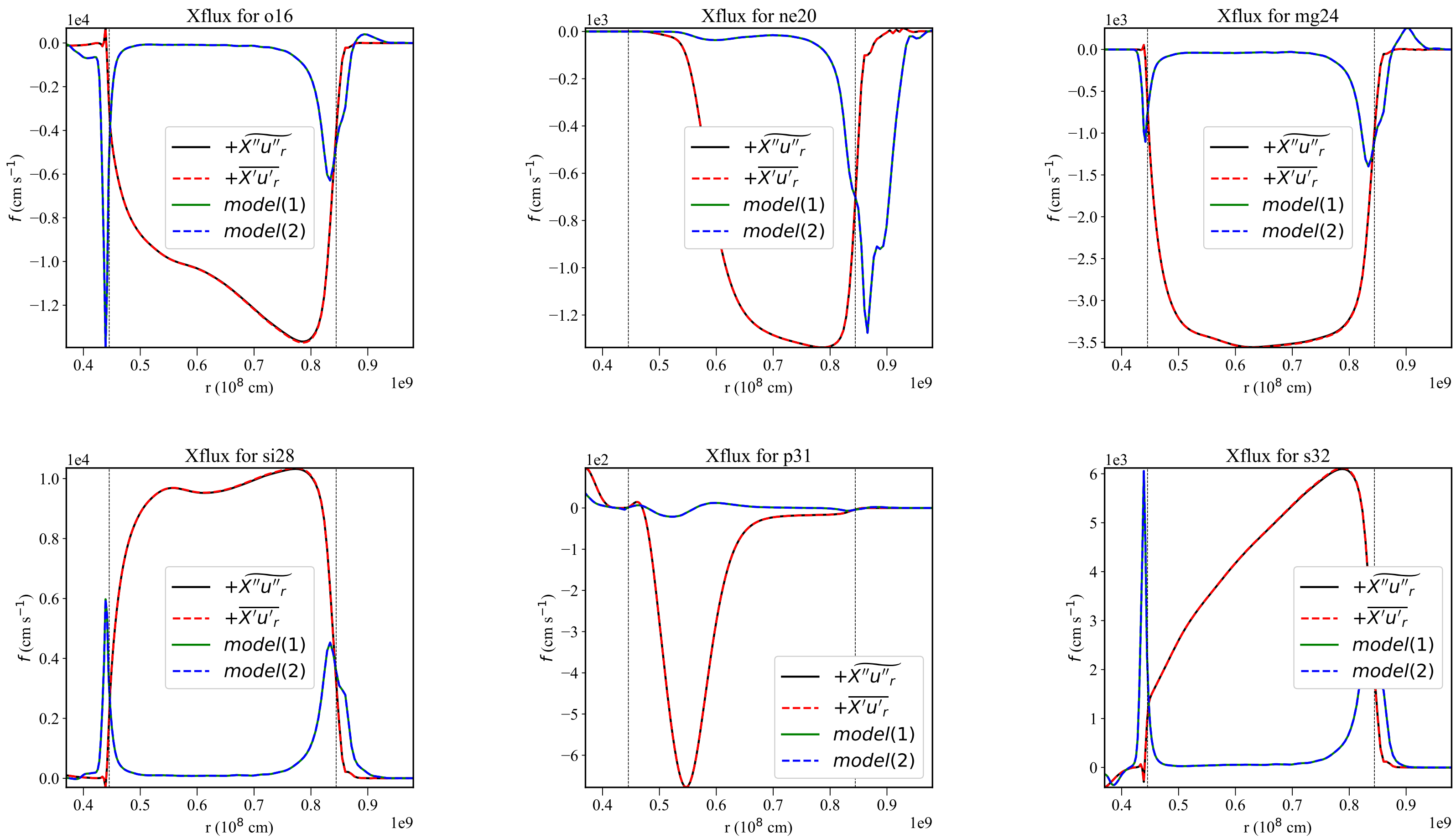
Models for radial composition flux:

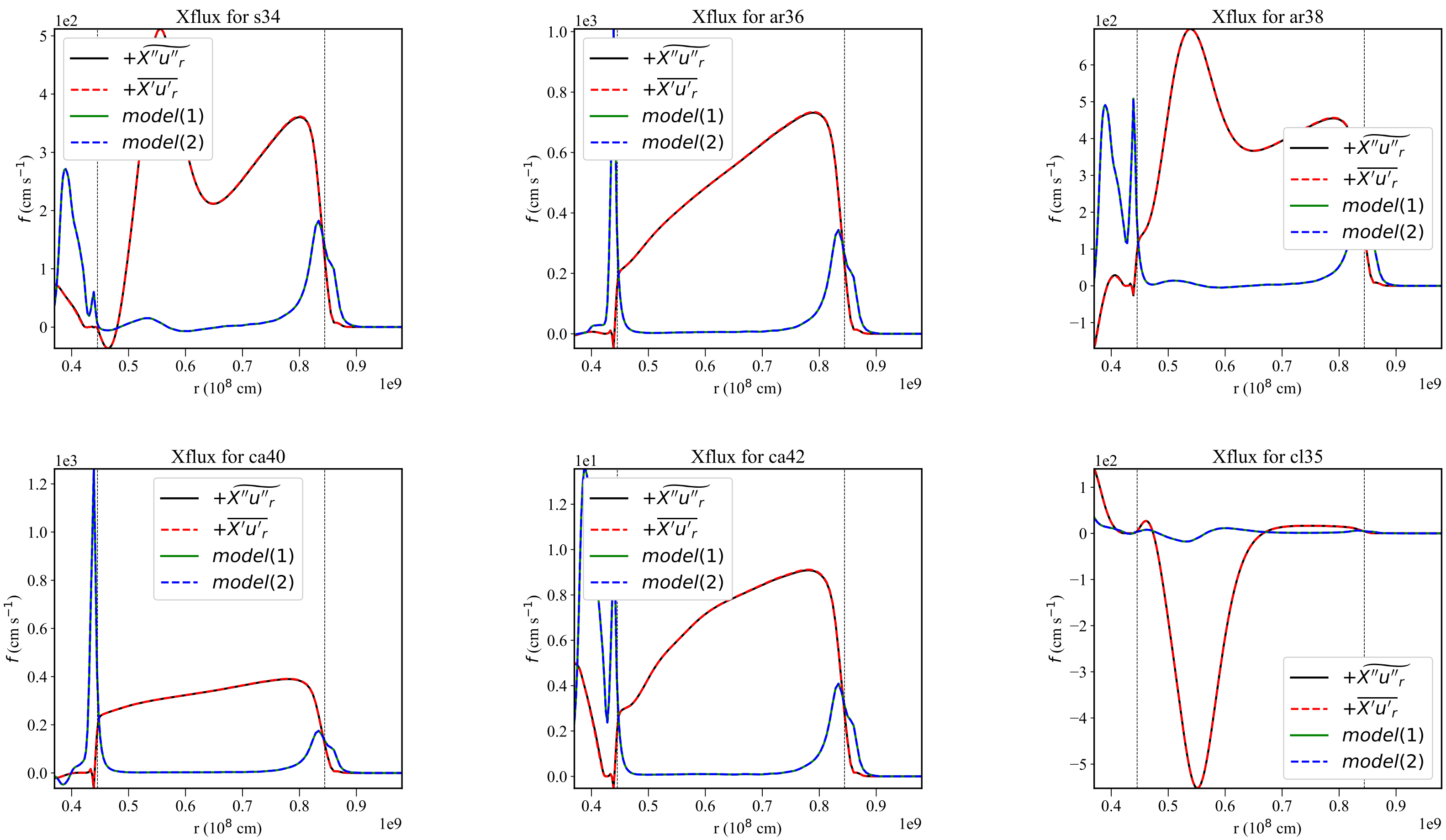
$$
\begin{aligned}
\overline{X'_\alpha u'_r} =&\ -D_{rr}\ \partial_r \overline{X}_\alpha = -\left[(\tau/C_D)\ \overline{u'_r u'_r} - S_{r\theta}\ \tau\ (\tau/C^2_D)\ \overline{u'_r u'_\theta}\right] \partial_r \overline{X}_\alpha \qquad \text{model (1)} \\
\overline{X'_\alpha u'_r} =&\ -D_{rr}\ \partial_r \overline{X}_\alpha = -\left[(\tau/C_D)\ \overline{u'_r u'_r} - S_{r\phi}\ \tau\ (\tau/C^2_D)\ \overline{u'_r u'_\phi}\right] \partial_r \overline{X}_\alpha \qquad \text{model (2)}
\end{aligned}
$$

[4]No idea how they did that, but the algebra must have been brutal.

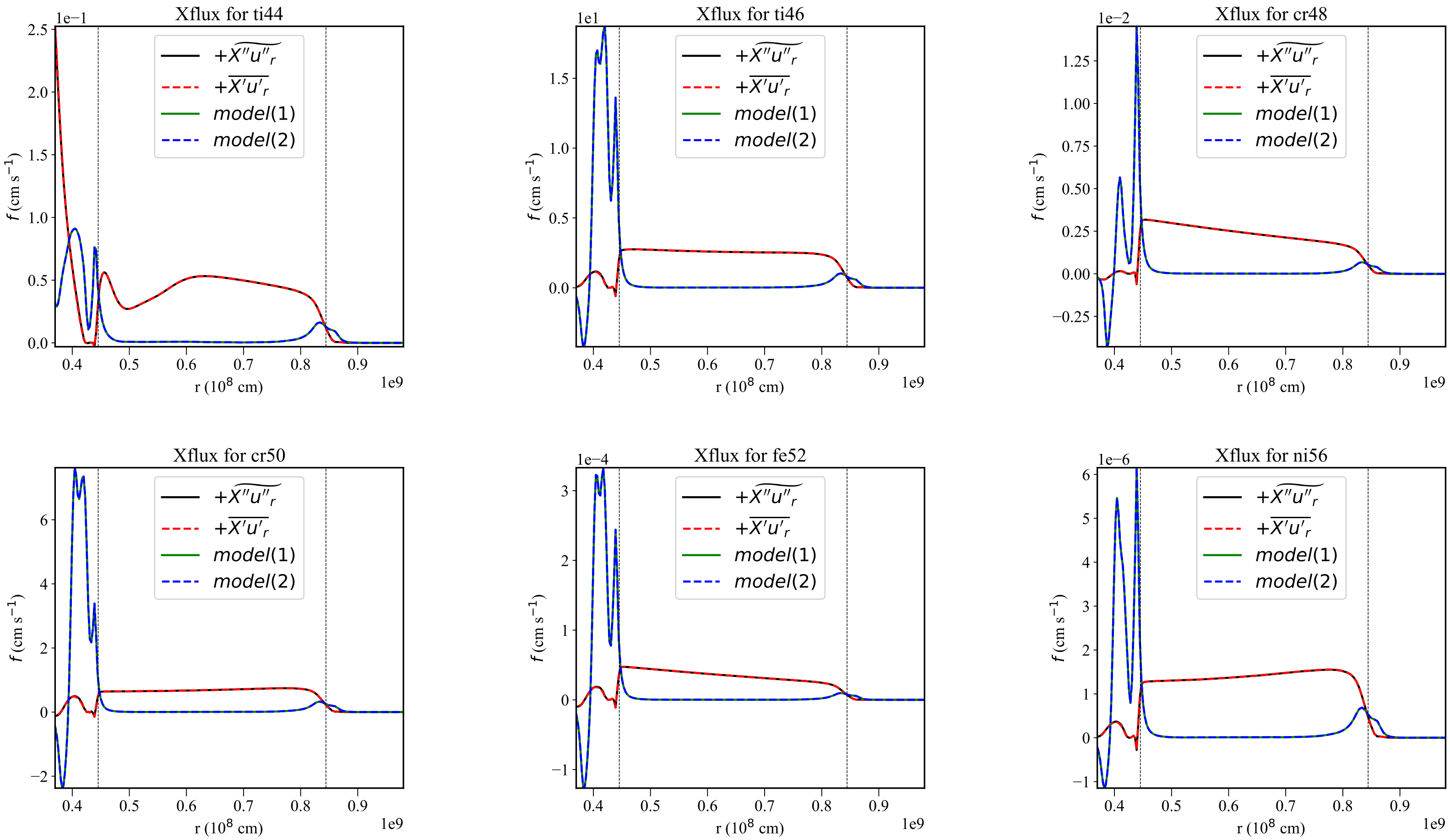
Results (based on oburn lrez data):

$$\overline{X'_\alpha u'_r} \sim \widetilde{X''_\alpha u''_r} \neq -D_{rr}\,\partial_r \overline{X}_\alpha = -\left[(\tau/C_D)\,\overline{u'_r u'_r} - \cancel{S\,\tau\,(\tau/C_D^2)\,\overline{u'_r u'_\theta}} \right]^{<<\,(\tau/C_D)\,\overline{u'_r u'_r}} \partial_r \overline{X}_\alpha \sim -(\tau/C_D)\,\overline{u'_r u'_r}\partial_r \overline{X}_\alpha$$





Xflux for s34
Xflux for ar36
Xflux for ar38
Xflux for ca40
Xflux for ca42
Xflux for cl35
$+\widetilde{X''u''_r}$
$+\overline{X'u'_r}$
$model(1)$
$model(2)$
f (cm s^{-1})
r (10^8 cm)
1e9
1e2
1e3
1e1


Xflux for ti44
Xflux for ti46
Xflux for cr48
Xflux for cr50
Xflux for fe52
Xflux for ni56
$+\widetilde{X''u''_r}$
$+\overline{X'u'_r}$
$model(1)$
$model(2)$
f (cm s^{-1})
r (10^8 cm)
1e9

2 Governing equations for inhomogeneous, compressible and adiabatic flow with gravity in stars and its passive/active scalar turbulent flux

$$\partial_r \overline{m} = -\overline{\rho}\ \overline{m}\ \overline{g}_r/\Gamma_1 \overline{P} + 4\pi r^2 \overline{\rho} \tag{7}$$

$$\partial_r \overline{P} = -\overline{\rho}\ \overline{g}_r \tag{8}$$

$$\partial_r \widetilde{L} = -4\pi r^2 \widetilde{u}_r \overline{\rho}\ \overline{g}_r/\Gamma_1 + \widetilde{\epsilon}_t \partial_r 4\pi r^2 \overline{\rho} \widetilde{u}_r \tag{9}$$

$$\partial_r \overline{T} = -(\Gamma_3 - 1)\ \overline{\rho}\ \overline{T}\ \overline{g}_r/\Gamma_1 \overline{P} \tag{10}$$

$$\partial_t \widetilde{X}_\alpha = \widetilde{\dot{X}}_\alpha^{nuc} - (1/\overline{\rho}) \nabla_r \overline{\rho} \widetilde{X''_\alpha u''_r} - \widetilde{u}_r \partial_r \widetilde{X}_i \tag{11}$$

$$\partial_t \widetilde{X''_\alpha u''_r} = -(1/\overline{\rho}) \nabla_r \overline{\rho X''_\alpha u''_r u''_r} - \nabla_r \widetilde{u}_r \widetilde{X''_\alpha u''_r} - \widetilde{u''_r u''_r} \partial_r \widetilde{X}_\alpha - (1/\overline{\rho}) \overline{X''_\alpha \partial_r P} + (1/\overline{\rho}) \overline{u''_r \rho \dot{X}_\alpha^{\mathrm{nuc}}} + (1/\overline{\rho}) \mathcal{G}_\alpha \tag{12}$$

2.1 Turbulent scalar flux models derivation

t.b.d.

References

Michael M Rogers, Nagi N Mansour, and William C Reynolds. An algebraic model for the turbulent flux of a passive scalar. *Journal of Fluid Mechanics*, 203:77–101, 1989.

Table 1: Definitions:

ρ density	g_r radial gravitational acceleration
$m = \rho V = \rho \frac{4}{3}\pi r^3$ mass	$M = \int \rho(r) dV = \int \rho(r) 4\pi r^2 dr$ integrated mass
T temperature	$\mathcal{S} = \rho \epsilon_{\rm nuc}(q)$ nuclear energy production (cooling function)
P pressure	$\tau_{ij} = 2\mu S_{ij}$ viscous stress tensor (μ kinematic viscosity)
u_r, u_θ, u_ϕ velocity components	$S_{ij} = (1/2)(\partial_i u_j + \partial_j u_i)$ strain rate
$\mathbf{u} = u(u_r, u_\theta, u_\phi)$ velocity	$\widetilde{R}_{ij} = \overline{\rho} \widetilde{u''_i u''_j}$ Reynolds stress tensor
$j_z = r \sin\theta \ u_\phi$ specific angular momentum	$F_T = \chi \partial_r T$ heat flux
$d = \nabla \cdot \mathbf{u}$ dilatation	$\Gamma_1 = (d \ ln \ P / d \ ln \ \rho)\vert_s$
ϵ_I specific internal energy	$\Gamma_2/(\Gamma_2 - 1) = (d \ ln \ P / d \ ln \ T)\vert_s$
h specific enthalpy	$\Gamma_3 - 1 = (d \ ln \ T / d \ ln \ \rho)\vert_s$
$k = (1/2)\widetilde{u''_i u''_i}$ turbulent kinetic energy	$\widetilde{k}^r = (1/2)\widetilde{u''_r u''_r} = (1/2)\widetilde{R}_{rr}/\overline{\rho}$ radial turbulent kinetic energy
ϵ_k specific kinetic energy	$\widetilde{k}^\theta = (1/2)\widetilde{u''_\theta u''_\theta} = (1/2)\widetilde{R}_{\theta\theta}/\overline{\rho}$ angular turbulent kinetic energy
ϵ_t specific total energy	$\widetilde{k}^\phi = (1/2)\widetilde{u''_\phi u''_\phi} = (1/2)\widetilde{R}_{\phi\phi}/\overline{\rho}$ angular turbulent kinetic energy
s specific entropy	$\widetilde{k}^h = \widetilde{k}^\theta + \widetilde{k}^\phi$ horizontal turbulent kinetic energy
$v = 1/\rho$ specific volume	$f_k = (1/2)\overline{\rho} \widetilde{u''_i u''_i u''_r}$ turbulent kinetic energy flux
X_α mass fraction of isotope α	$f_k^r = (1/2)\overline{\rho} \widetilde{u''_r u''_r u''_r}$ radial turbulent kinetic energy flux
$\dot{X}_\alpha^{nuc}$ rate of change of X_α	$f_k^\theta = (1/2)\overline{\rho} \widetilde{u''_\theta u''_\theta u''_r}$ angular turbulent kinetic energy flux
A_α number of nucleons in isotope α	$f_k^\phi = (1/2)\overline{\rho} \widetilde{u''_\phi u''_\phi u''_r}$ angular turbulent kinetic energy flux
Z_α charge of isotope α	$f_k^h = f_k^\theta + f_k^\phi$ horizontal turbulent kinetic energy flux
A mean number of nucleons per isotope	$W_p = \overline{P' d''}$ turbulent pressure dilatation
Z mean charge per isotope	$W_b = \overline{\rho} \overline{u''_r} \widetilde{g}_r$ buoyancy
$f_P = \overline{P' u'_r}$ acoustic flux	$f_T = -\overline{\chi \partial_r T}$ heat flux (χ thermal conductivity)