Transport and nuclear burning during convective-reactive events in stars based on RANS analysis

Miroslav Mocák

(Collaborators: Simon Campbell, Casey Meakin, Dave Arnett, Cyril Georgy)

miroslav.mocak@gmail.com, ransx@googlegroups.com

Hydro Convective-Reactive Workshop Frankfurt 2019

Convective-Reactive Events

- occurs when timescales for nuclear reactions become comparable to transport timescales
- composition is significantly modified by nuclear reactions
- transport of chemical elements during such events can not be modelled by commonly used diffusion approximation anymore (if at all, convection is intrinsically a transport, not a diffusion)
- depending on the temperature and density distribution, the interplay between nuclear burning and transport leads to a fine structure of nuclear burning zones in stars (individual nuclear elements being burned or produced in shallow or deeper layers overlaying each other within a single convective region)
- to get this right is essential, because in reactive flows like core convection in stars, mixing controls rate of nuclear reactions, and eventually stellar yields

Reynolds-averaging (i.e. RANS analysis)

- Theory: Reynolds and Favrian decomposition

$$A(r,\theta,\phi) = \overline{A}(r) + A'(r,\theta,\phi) \qquad \overline{A(r)} = \frac{1}{\Delta T \Delta\Omega}\int_{\Delta T}\int_{\Delta\Omega} A(r,\theta,\phi)\, dt\, d\Omega$$

$$F(r,\theta,\phi) = \widetilde{F}(r) + F''(r,\theta,\phi) \qquad \widetilde{F} = \overline{\rho F}/\overline{\rho}$$

$$\underbrace{\overline{u}_r}_{\text{mean velocity}} = \underbrace{\widetilde{u}_r}_{\text{expansion velocity } \partial_t M/4\pi r^2 \overline{\rho}} - \underbrace{\overline{u''}_r}_{\text{turbulent mass flux } -\overline{\rho' u'_r}/\overline{\rho}}$$

  - https://github.com/mmicromegas/ransX/tree/master/DOCS

- Application: Any hydrodynamic equation
- >> Example: continuity equation for chemical elements

$$\partial_t(\rho X_i) = -\nabla \cdot (\rho \mathbf{u} X_i) + \rho \dot{X}_i^{\mathrm{nuc}}$$ < original equation

$$\partial_t \widetilde{X}_i = \widetilde{\dot{X}}_i^{nuc} - (1/\overline{\rho})\nabla_r f_i - \widetilde{u}_r \partial_r \widetilde{X}_i$$ < equivalent RANS equation, where $f_i = \overline{\rho}\widetilde{X''_i u''_r}$ is composition flux

NUCLEAR BURNING

COMPOSITION TRANSPORT

ADVECTION DUE TO BACKGROUND EXPANSION

Stellar structure equations (for adiabatic convection, no rotation, no magnetic fields)

- where does the composition transport equations fall in the global picture of stellar structure evolution equations and what we can improve by looking at hydro through RANS lens?

$$
\begin{aligned}
\partial_r M &= +\, 4\pi r^2 \rho \\
\partial_r P &= -\, \rho g_r - \rho \partial_t \widetilde{u} \\
\partial_r L &= +\, 4\pi r^2 \left(\epsilon_{nuc} - \epsilon_\nu - c_P \partial_t T + (\delta/\rho)\partial_t P\right) \\
\partial_r T &= +\, T g_r \nabla_{ad}/P \\
\partial_t X_i &= +\, \dot{X}_i^{nuc} - \boxed{(1/\overline{\rho})\nabla_r f_i} - \widetilde{u}_r \partial_r \widetilde{X}_i
\end{aligned}
$$

Stellar structure equations (no rotation, no magnetic fields)

- where does the composition transport equations fall in the global picture of stellar structure evolution equations and what we can improve by looking at hydro through RANS lens?

$$\partial_r \overline{m} = 4\pi r^2 \overline{\rho} + (4\pi r^3/3\widetilde{u}_r)\left[-\nabla_r f_\rho + (f_\rho/\overline{\rho})\partial_r\overline{\rho} - \overline{\rho}\overline{d} - \partial_t\overline{\rho}\right]$$

$$\partial_r \overline{P} = \overline{\rho}\overline{g} - \overline{\rho}\partial_t\widetilde{u}_r - \nabla_r\widetilde{R}_{rr} - \overline{G}^M_r - \overline{\rho}\widetilde{u}_r\partial_r\widetilde{u}_r$$

$$\partial_r\widetilde{L} = 4\pi r^2\overline{\rho}\widetilde{\epsilon}_{nuc} + 4\pi r^2\left[-\nabla_r(f_i+f_{th}+f_K+f_p) - \overline{Pd} - \widetilde{R}_{ir}\partial_r\widetilde{u}_i + W_b + \overline{\rho}\widetilde{D}_t\widetilde{u}_i\widetilde{u}_i/2 - \overline{\rho}\partial_t\widetilde{\epsilon}_t\right] + \widetilde{\epsilon}_t\partial_r 4\pi r^2\overline{\rho}\widetilde{u}_r$$

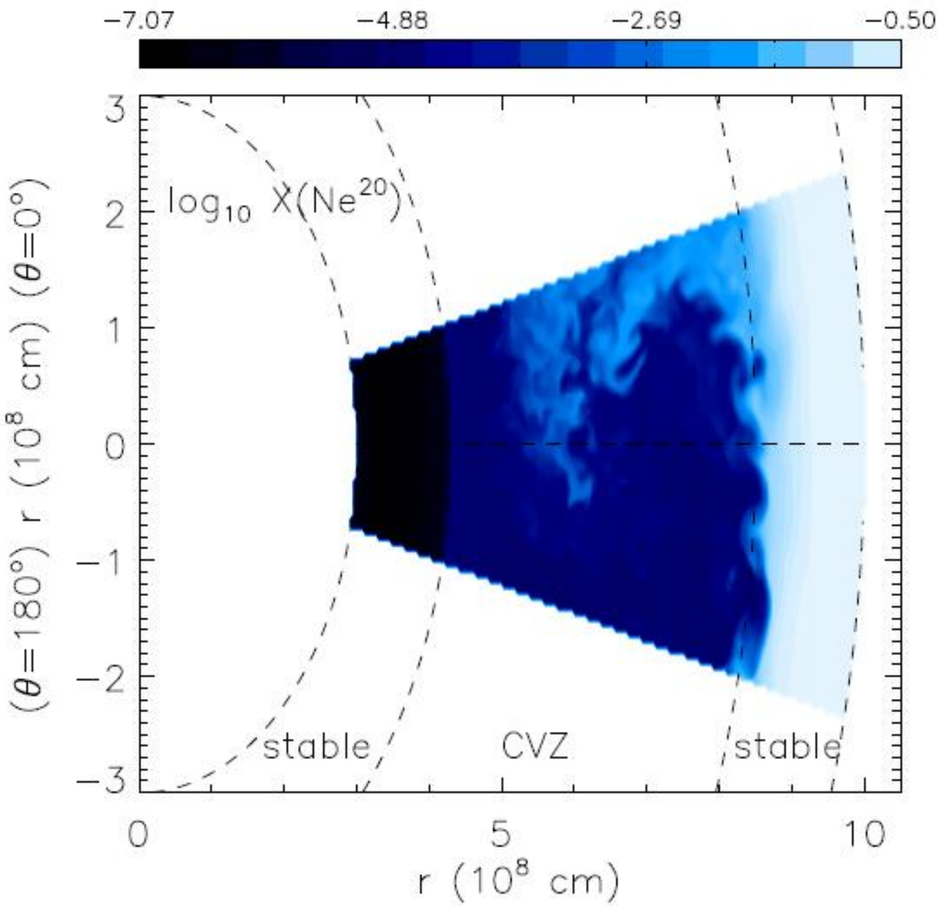
$$\partial_r\overline{T} = (1/\overline{u}_r)\left[-\nabla_r f_T + (1-\Gamma_3)\overline{T}\,\overline{d} + (2-\Gamma_3)\overline{T'd'} + \epsilon_{nuc}/c_v + \nabla\cdot f_{th}/(\rho c_v) - \partial_t T\right]$$

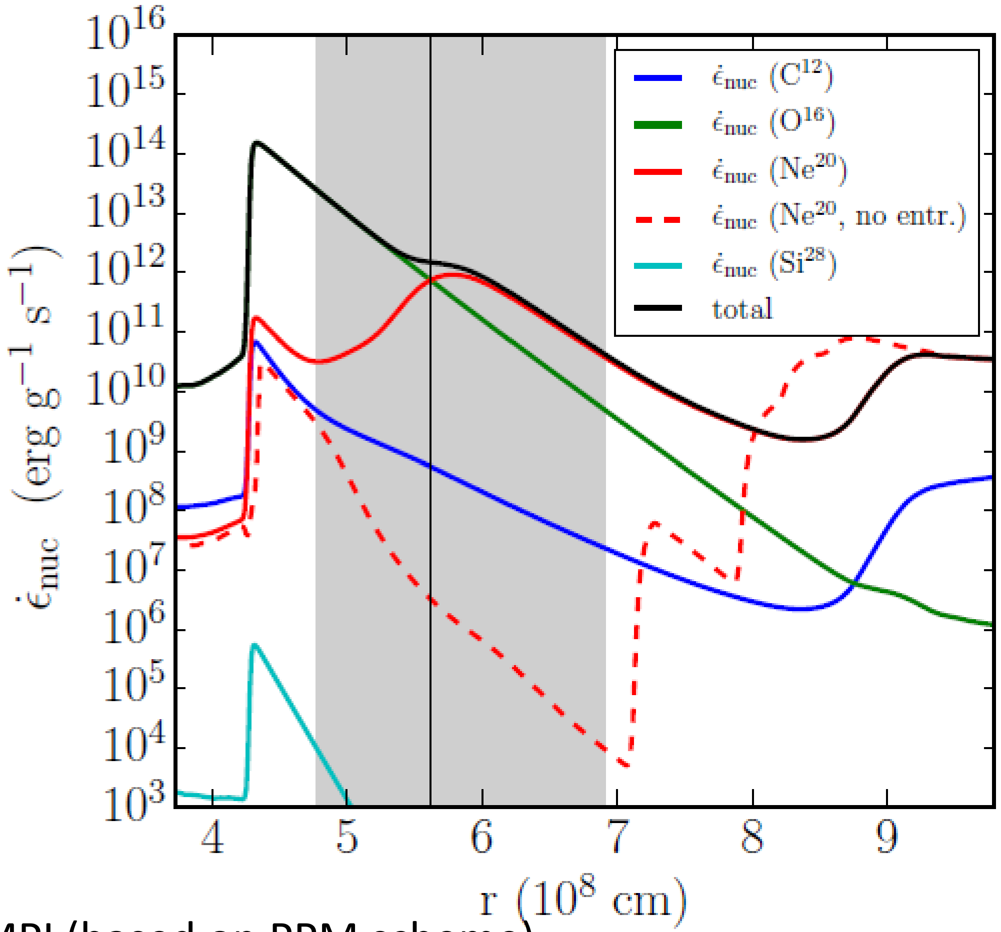
$$\partial_t\widetilde{X}_i = \widetilde{\dot{X}}_i^{nuc} - (1/\overline{\rho})\nabla_r f_i - \widetilde{u}_r\partial_r\widetilde{X}_i$$

Oxygen-Neon burning convective shell

2018MNRAS.481.2918M Mocák et al, 2018

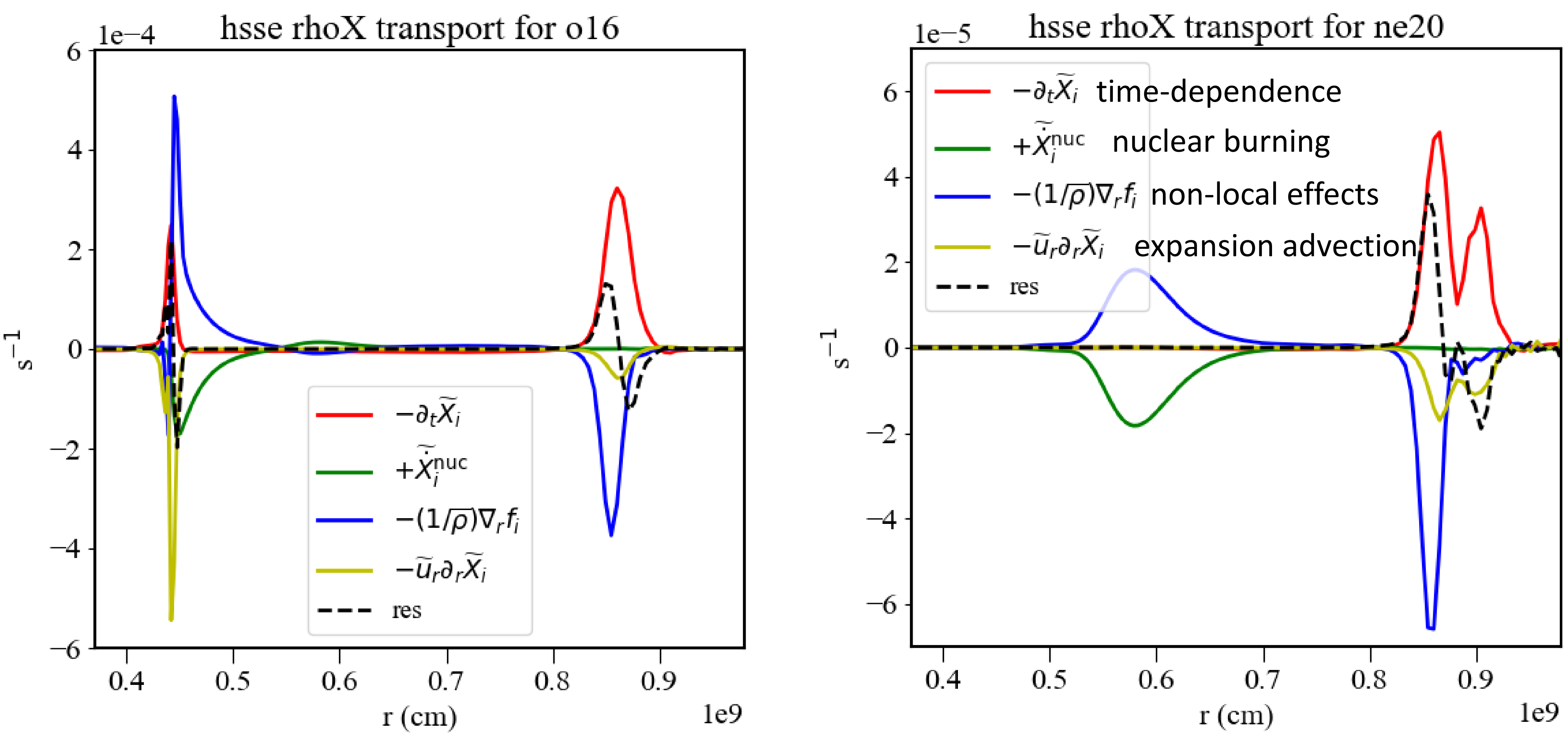
- multiple burning zones within single convection zone



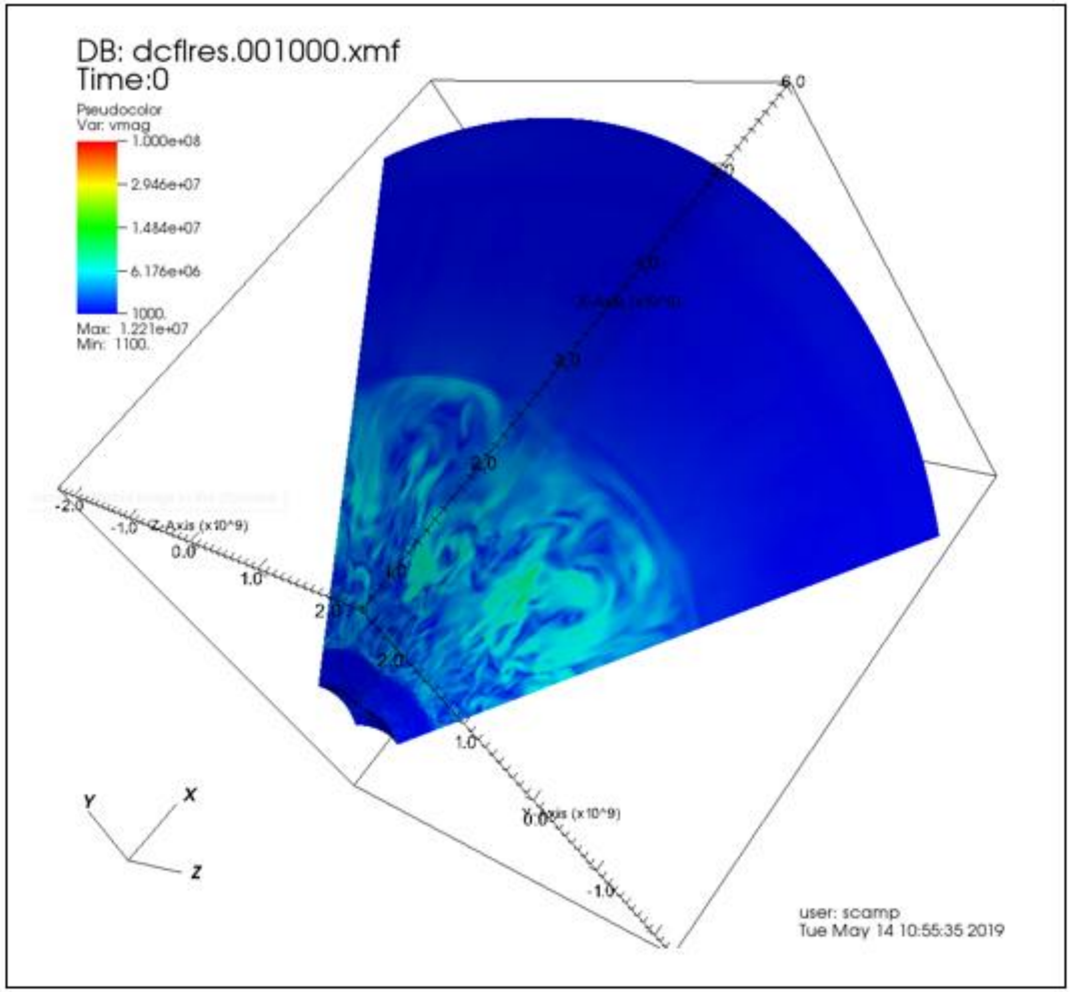


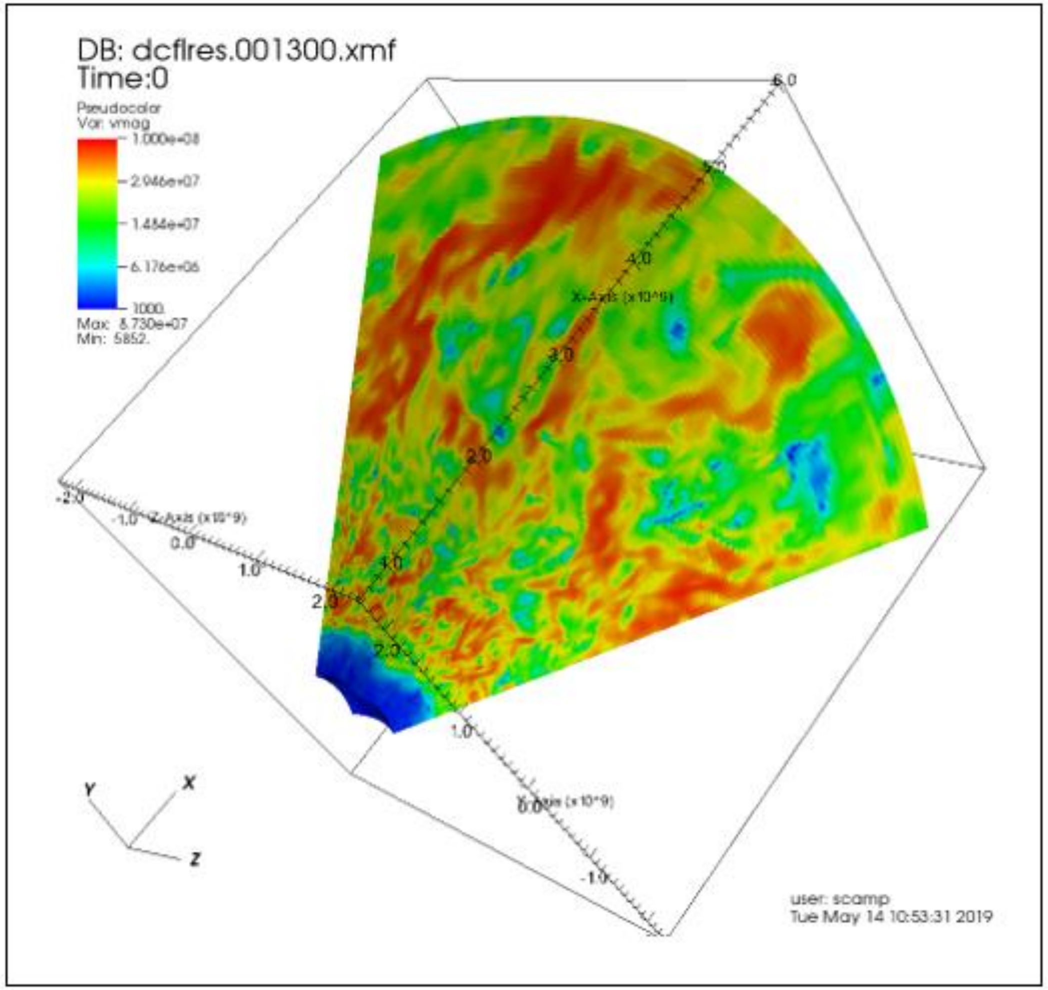
ILES simulation done by PROMPI (based on PPM scheme)

Transport and nuclear burning



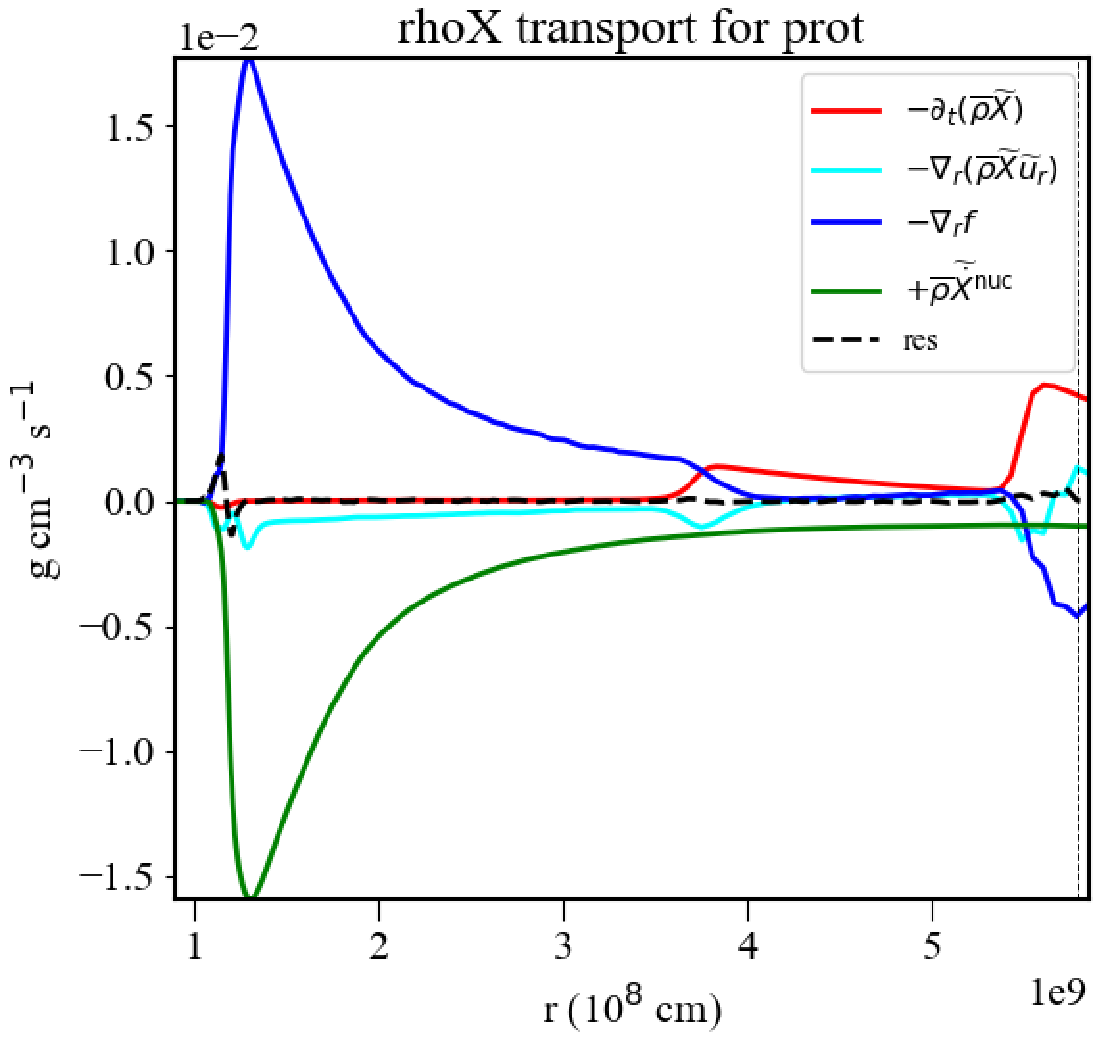
Dual core flash

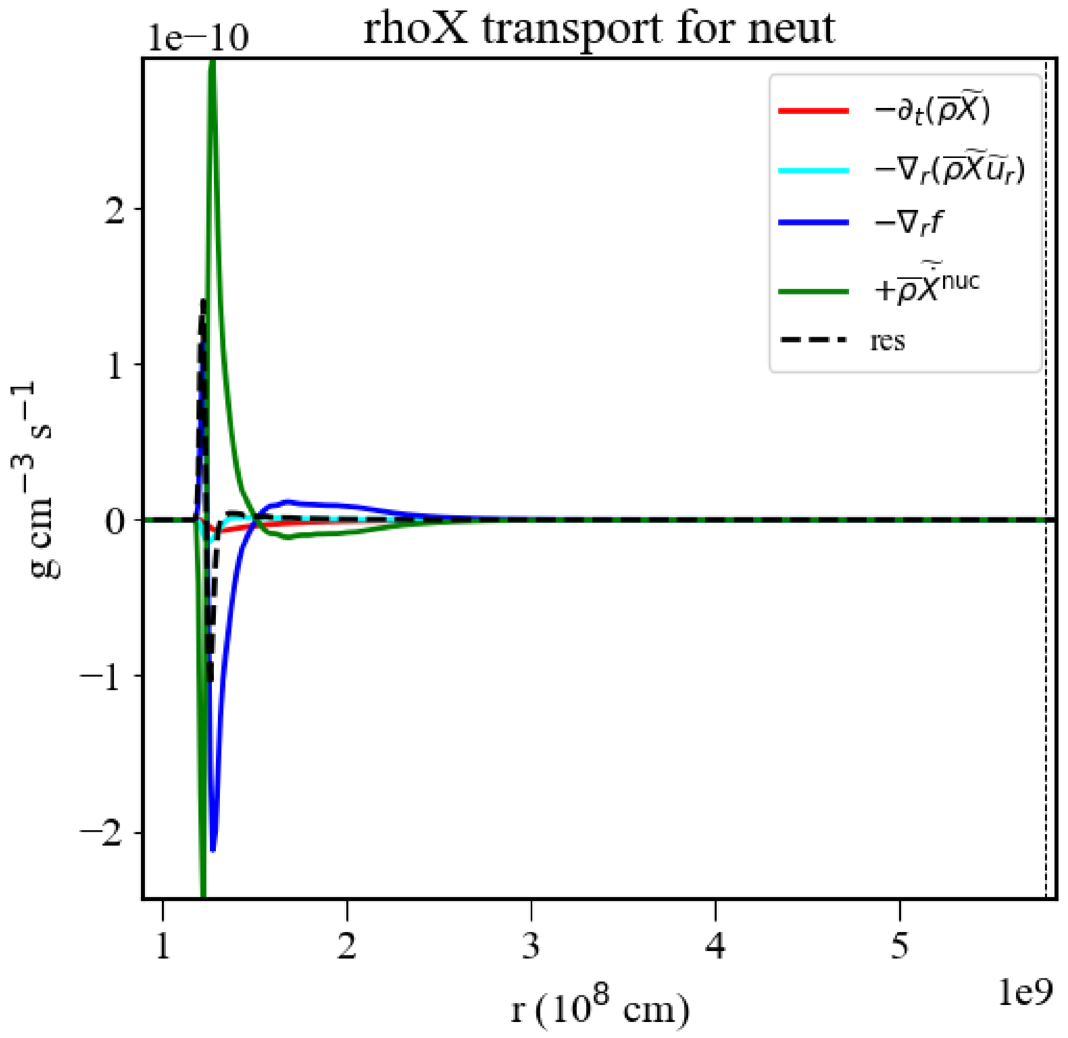




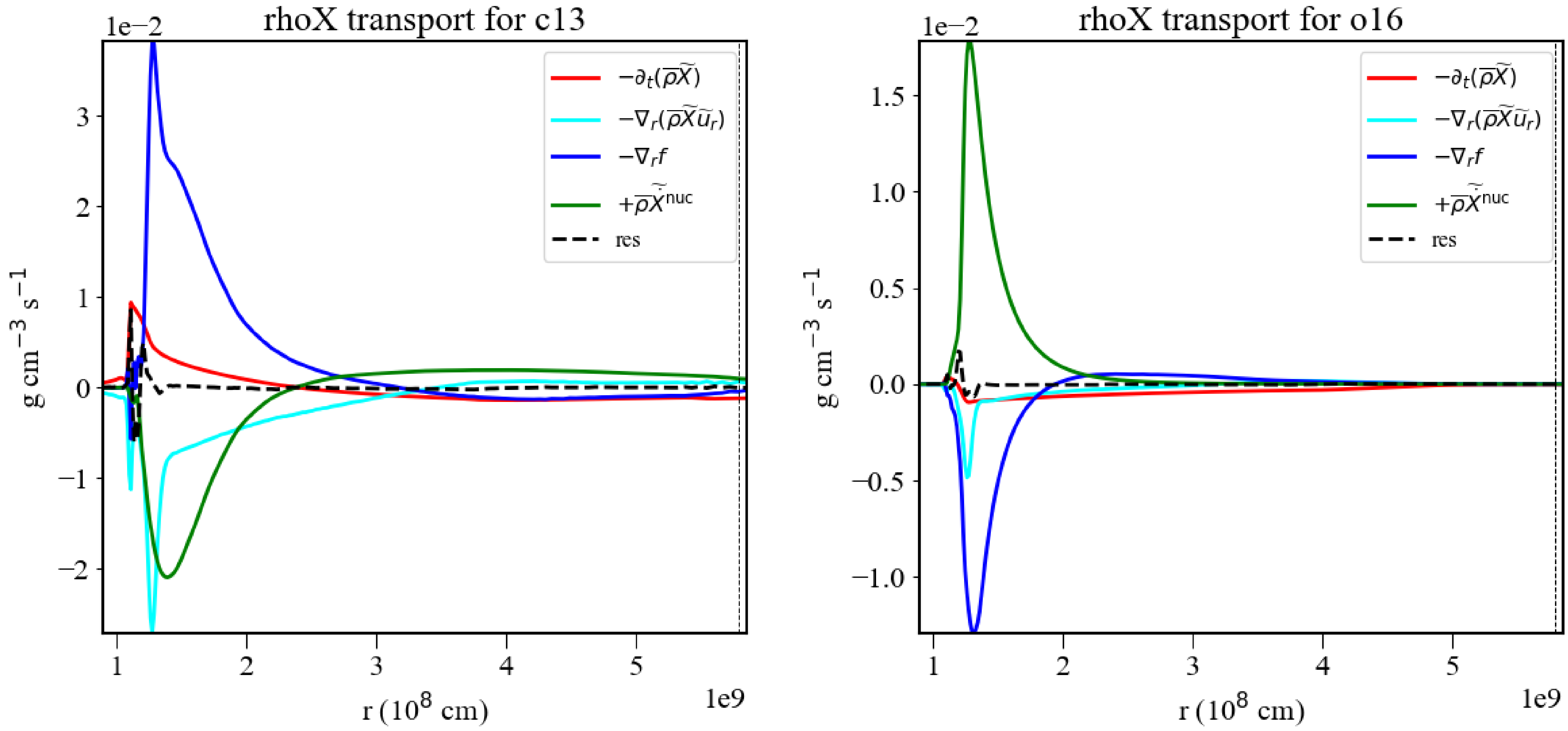
ILES simulation done by PROMPI (based on PPM scheme)

Transport and nuclear burning

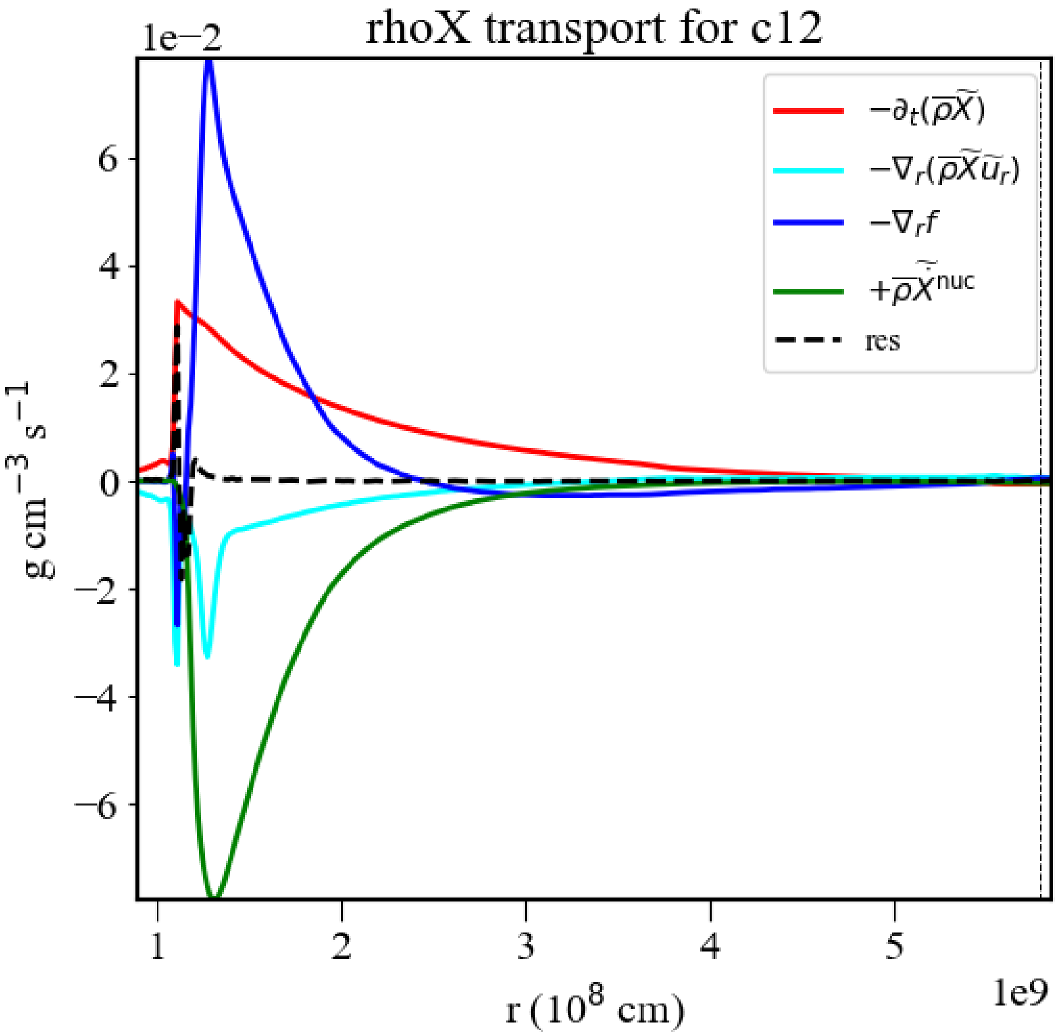


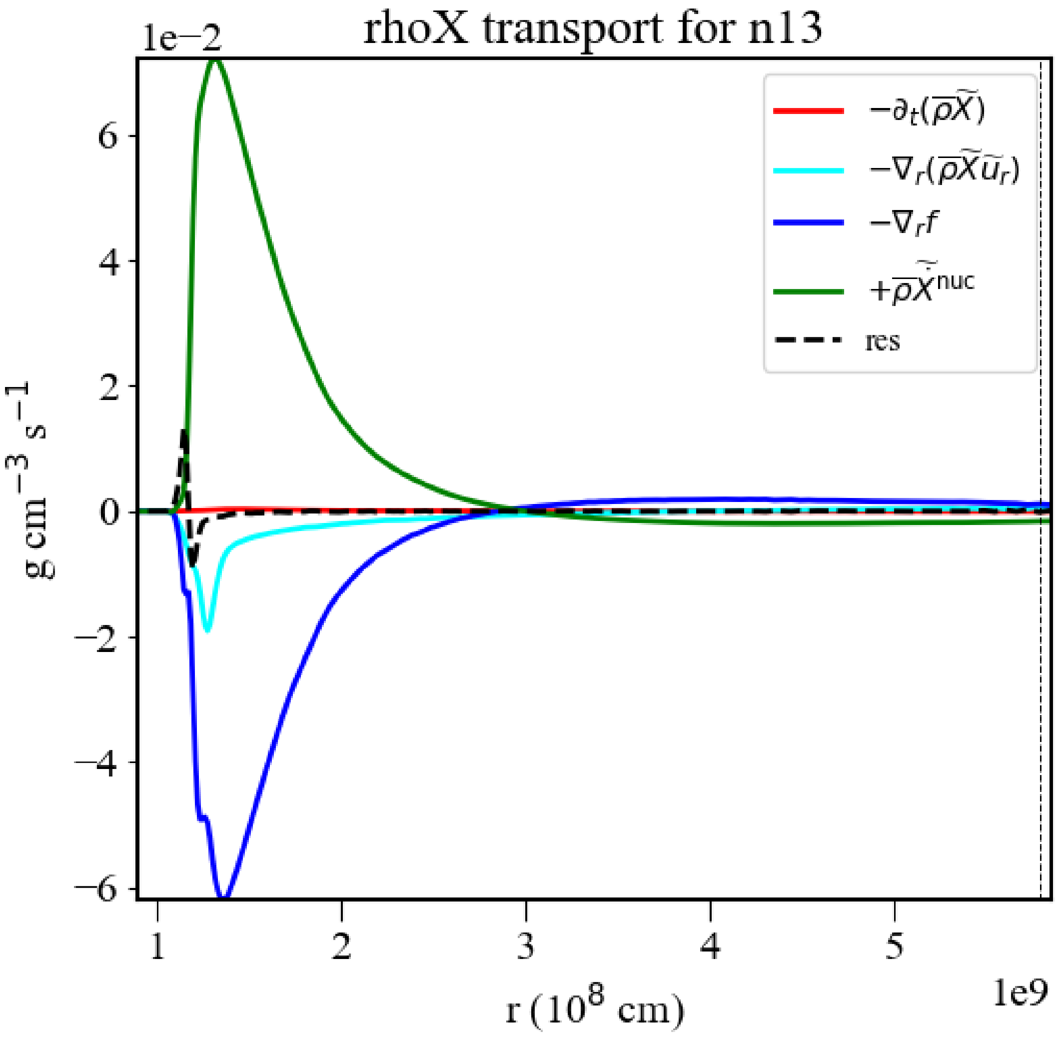


Transport and nuclear burning c13(alpha,n)o16



Transport and nuclear burning c12(p,gamma)n13





How to model turbulent composition flux
(or any flux)

- Local (diffusion-like) models for terms in zero-order moments (e.g. MLT diffusion approximation to turbulent composition flux for the composition evolution equation: zero-order moment equation)

- Local (diffusion-like) models for terms in second-order moments (e.g Biferale et al. (2011): diffusion approximation to higher order terms in the turbulent composition flux evolution equation: second-order moment equation)

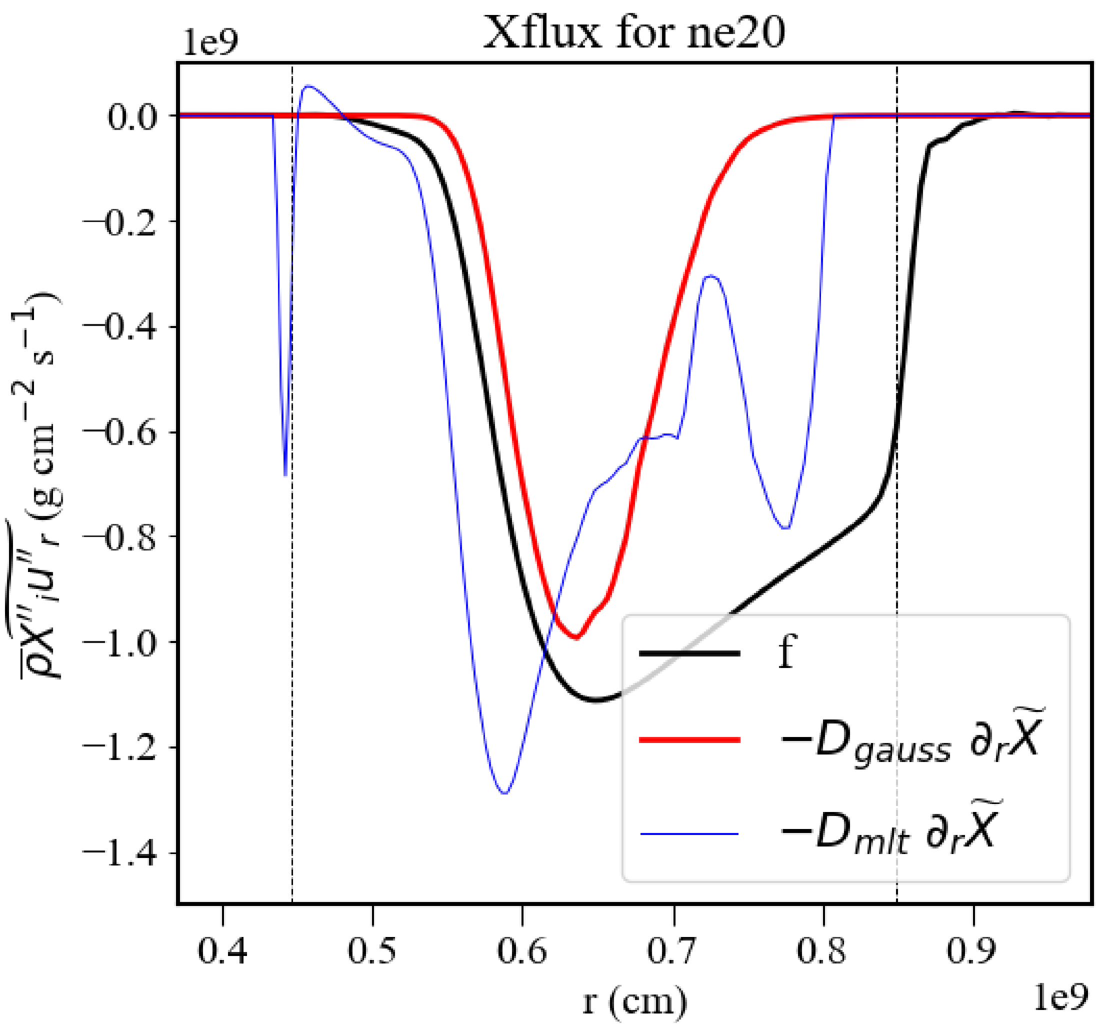
- Algebraic models (e.g. Rogers et al. (1989): identification of dominant terms in the composition flux equation and based on them, derivation of a model for the flux using algebraic manipulation)

Local (diffusion) models of composition flux

$$\partial_r M = + 4\pi r^2 \rho$$
$$\partial_r P = - \rho g_r - \rho \partial_t \widetilde{u}$$
$$\partial_r L = + 4\pi r^2 \left(\epsilon_{nuc} - \epsilon_\nu - c_P \partial_t T + (\delta/\rho)\partial_t P\right)$$
$$\partial_r T = + T g_r \nabla_{ad}/P$$
$$\partial_t X_i = + \dot{X}_i^{nuc} - \boxed{(1/\overline{\rho})\nabla_r f_i} - \widetilde{u}_r \partial_r \widetilde{X}_i$$

where

$$f_i = - D \; \rho \; \partial_r \widetilde{X}_i$$
$$\widetilde{u}_r = - \dot{M}/4\pi r^2 \overline{\rho}$$



Local (diffusion-like) models for terms in composition flux evolution equation

$$
\begin{aligned}
\partial_r M &= +\, 4\pi r^2 \rho \\
\partial_r P &= -\, \rho g_r - \rho \partial_t \widetilde{u} \\
\partial_r L &= +\, 4\pi r^2 \left(\epsilon_{nuc} - \epsilon_\nu - c_P \partial_t T + (\delta/\rho)\partial_t P\right) \\
\partial_r T &= +\, T g_r \nabla_{ad}/P \\
\partial_t \widetilde{X}_i &= +\, \dot{X}_i^{nuc} - \boxed{(1/\overline{\rho})\nabla_r f_i} - \widetilde{u}_r \partial_r \widetilde{X}_i \\
\overline{\rho}\partial_t (f_i/\overline{\rho}) &= -\, \nabla_r f_i^r - f_i \partial_r \widetilde{u}_r - \widetilde{R}_{rr}\partial_r \widetilde{X}_i - \overline{X_i'' \partial_r P} \\
&\quad + \overline{u_r'' \rho \dot{X}_i^{\mathrm{nuc}}} + \mathcal{G}_i - \overline{\rho}\widetilde{u}_r \partial_r f_i/\overline{\rho}
\end{aligned}
$$

where

$$
\begin{aligned}
f_i^r &= -\, D\partial_r f_i \\
\widetilde{R}_{rr} &= +\, \mathrm{model}_{rxx} \\
\overline{X_i'' \partial_r P} &= +\, \mathrm{model}_{xgrp} \\
\overline{u_r'' \rho \dot{X}_i^{\mathrm{nuc}}} &= +\, \mathrm{model}_{udxn} \\
\mathcal{G}_i &\sim 0 \\
\widetilde{u}_r &= -\, \dot{M}/4\pi r^2 \overline{\rho}
\end{aligned}
$$

Algebraic models

$$\overline{\rho}\partial_t(f_i/\overline{\rho}) = -\nabla_r f_i^r - f_i\partial_r\widetilde{u}_r - \widetilde{R}_{rr}\partial_r\widetilde{X}_i - \overline{X_i''\partial_r P} + \overline{u_r''\rho\dot{X}_i^{\rm nuc}} + \mathcal{G}_i - \overline{\rho}\widetilde{u}_r\partial_r f_i/\overline{\rho}$$

$$\overline{\rho}\partial_t(f_i/\overline{\rho}) = -f_i\partial_r\widetilde{u}_r - \widetilde{R}_{rr}\partial_r\widetilde{X}_i + \psi_i \quad \text{where } \psi_i = -\nabla_r f_i^r - \overline{X_i''\partial_r P} + \overline{u_r''\rho\dot{X}_i^{\rm nuc}} + \mathcal{G}_i - \overline{\rho}\widetilde{u}_r\partial_r f_i/\overline{\rho}$$

$$0 = -f_i\partial_r\widetilde{u}_r - \widetilde{R}_{rr}\partial_r\widetilde{X}_i + \psi_i \quad \text{quasi-static flux}$$

$$0 = -f_i\partial_r\widetilde{u}_r - \widetilde{R}_{rr}\partial_r\widetilde{X}_i + (C_D/\tau)f_i \quad \text{assume model for } \psi_i = +(C_D/\tau)f_i$$

$$\mathcal{O}_r f_i = -\widetilde{R}_{rr}\partial_r\widetilde{X}_i \quad \text{where} \quad \mathcal{O}_r = C_D/\tau - \partial_r\widetilde{u}_r$$

$$\boxed{f_i = -\mathcal{O}_r^{-1}\widetilde{R}_{rr}\partial_r\widetilde{X}_i} \quad \text{algebraic model for turbulent flux}$$

where

$$f_i = +\overline{\rho}\widetilde{X_i''u_r''} \quad \text{composition flux for element } i$$

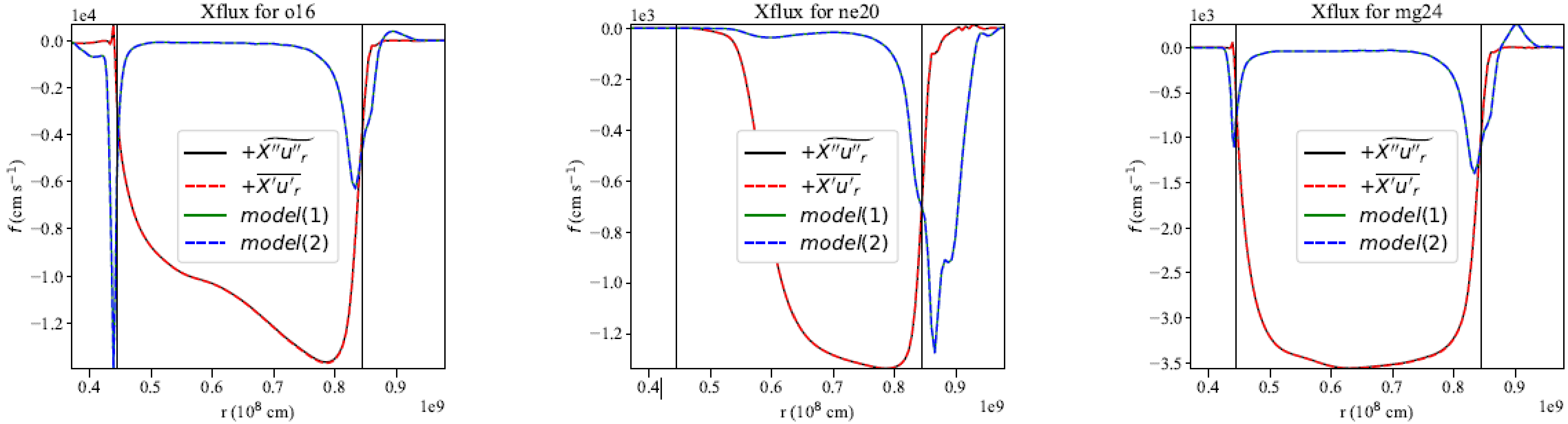
$$f_i^r = +\overline{\rho}\widetilde{X_i''u_r''u_r''} \quad \text{flux of composition flux}$$

$$\widetilde{R}_{rr} = +\overline{\rho}\widetilde{u_r''u_r''} \quad \text{Reynolds stress}$$

Algebraic models (for shear flow: Rogers 1989)

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

$$\overline{X'_\alpha u'_r} = -D_{rr}\,\partial_r \overline{X}_\alpha = -\left[(\tau/C_D)\,\overline{u'_r u'_r} - S_{r\phi}\,\tau\,(\tau/C_D^2)\,\overline{u'_r u'_\phi}\right]\partial_r \overline{X}_\alpha \qquad \text{model (2)}$$



Not working for stellar convection

Summary

- simple diffusion models to mixing during convective-reactive events do not work
- new mixing models are needed
- engineering approach based on the RANS analysis has potential to deliver us new mixing models either based on modeling the turbulent flux itself or by inventing closures for the turbulent flux evolution equation

(this has started to be feasible only now due to availability of 3D time-dependent multi-species hydrodynamic compressible simulations with nuclear burning at reasonable resolution covering multiple convective turnover timescales - in our case we use PROMPI code capable of calculation of Reynolds-averages at runtime and post-processing by open-source ransX framework https://github.com/mmicromegas/ransX)

Local (diffusion-like) models of composition flux

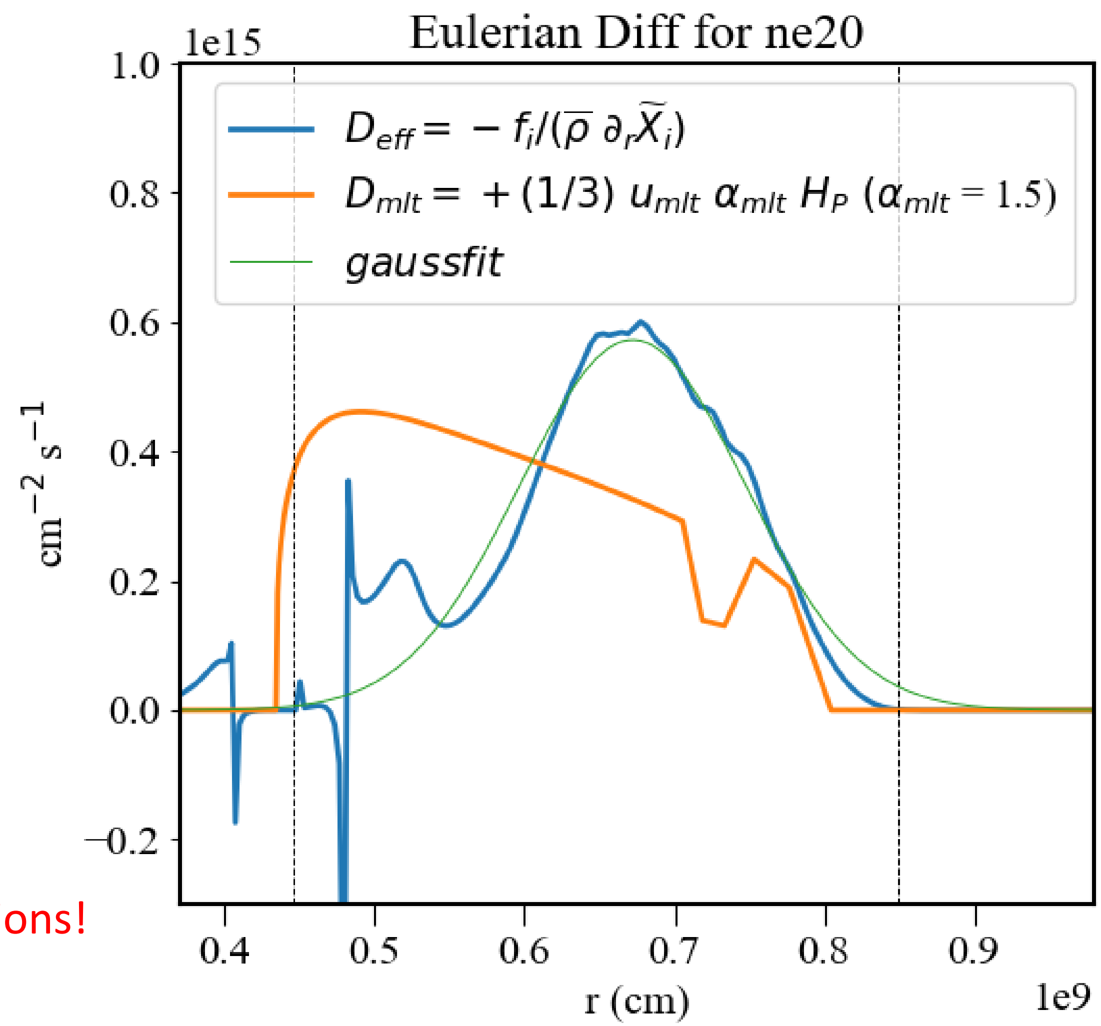
$$f_i = -D\ \overline{\rho}\ \partial_r \widetilde{X}_i$$

$$D_{mlt} = \frac{1}{3}\ u_{mlt}\ (\alpha H_P)$$

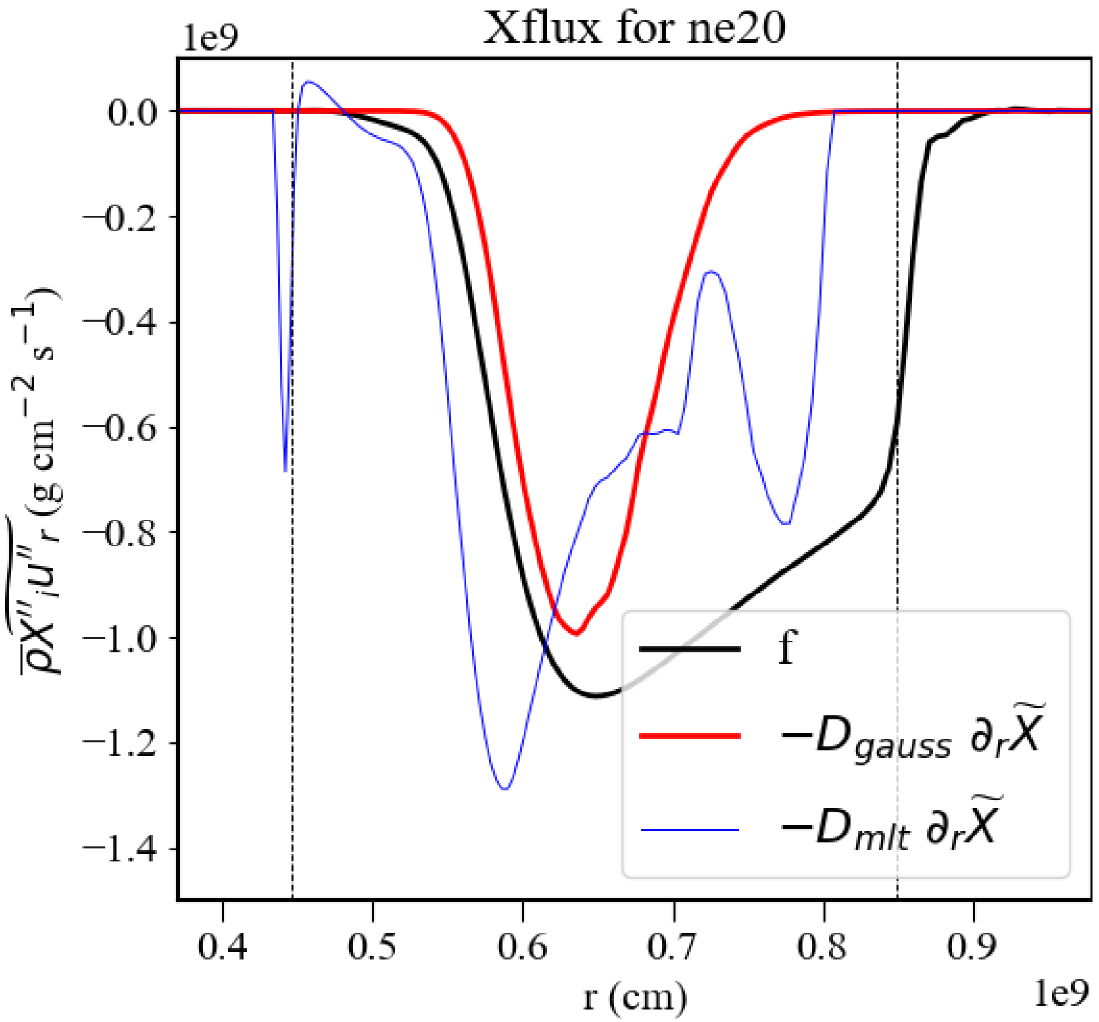
$$D_{eff} = -f_i/(\overline{\rho}\partial_r \widetilde{X}_i)$$

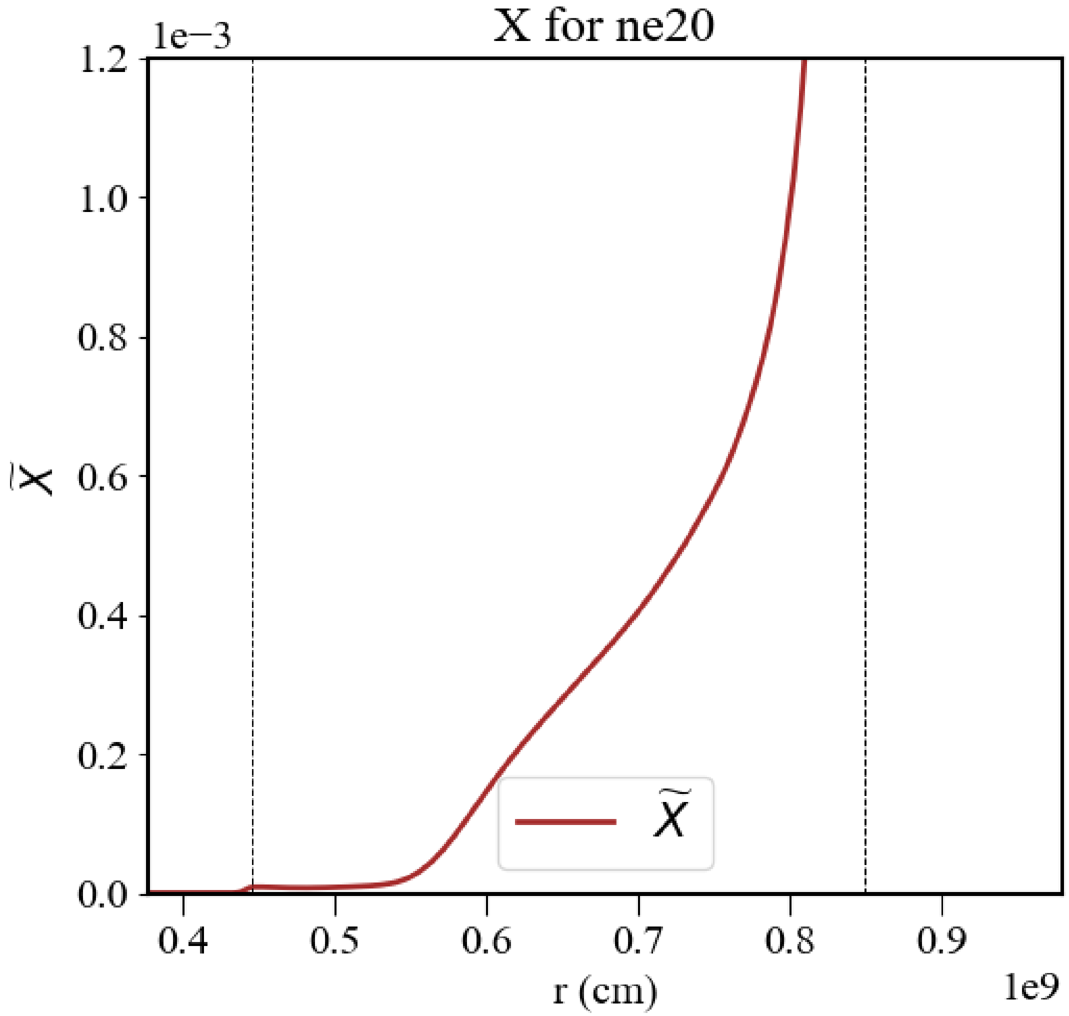
$$D_{gauss} = max(D_{mlt})\ e^{-\frac{(r-r_c^{middle})^2}{2\ width_c{}^2}}$$

To get this right is essential, because in reactive flows, mixing controls rate of nuclear reactions!

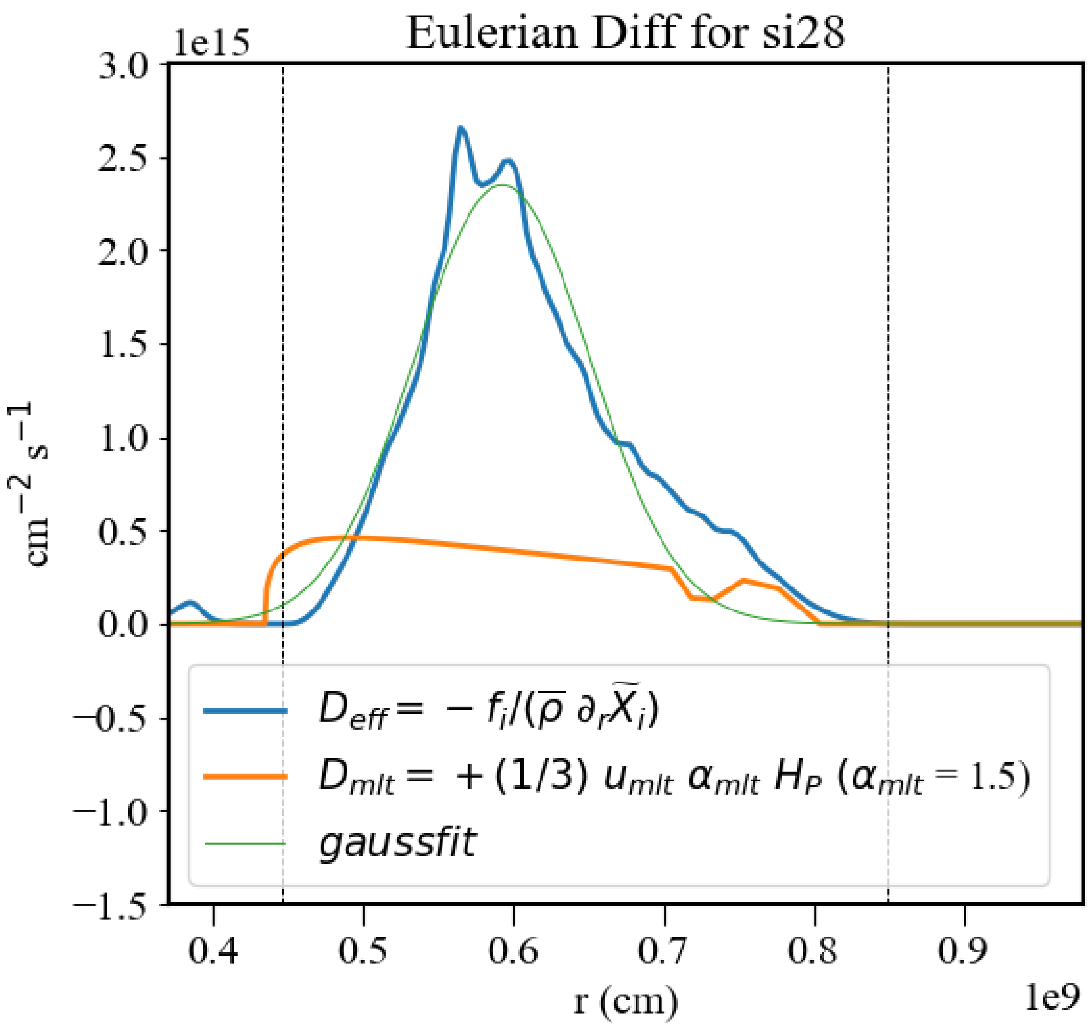


Composition flux model

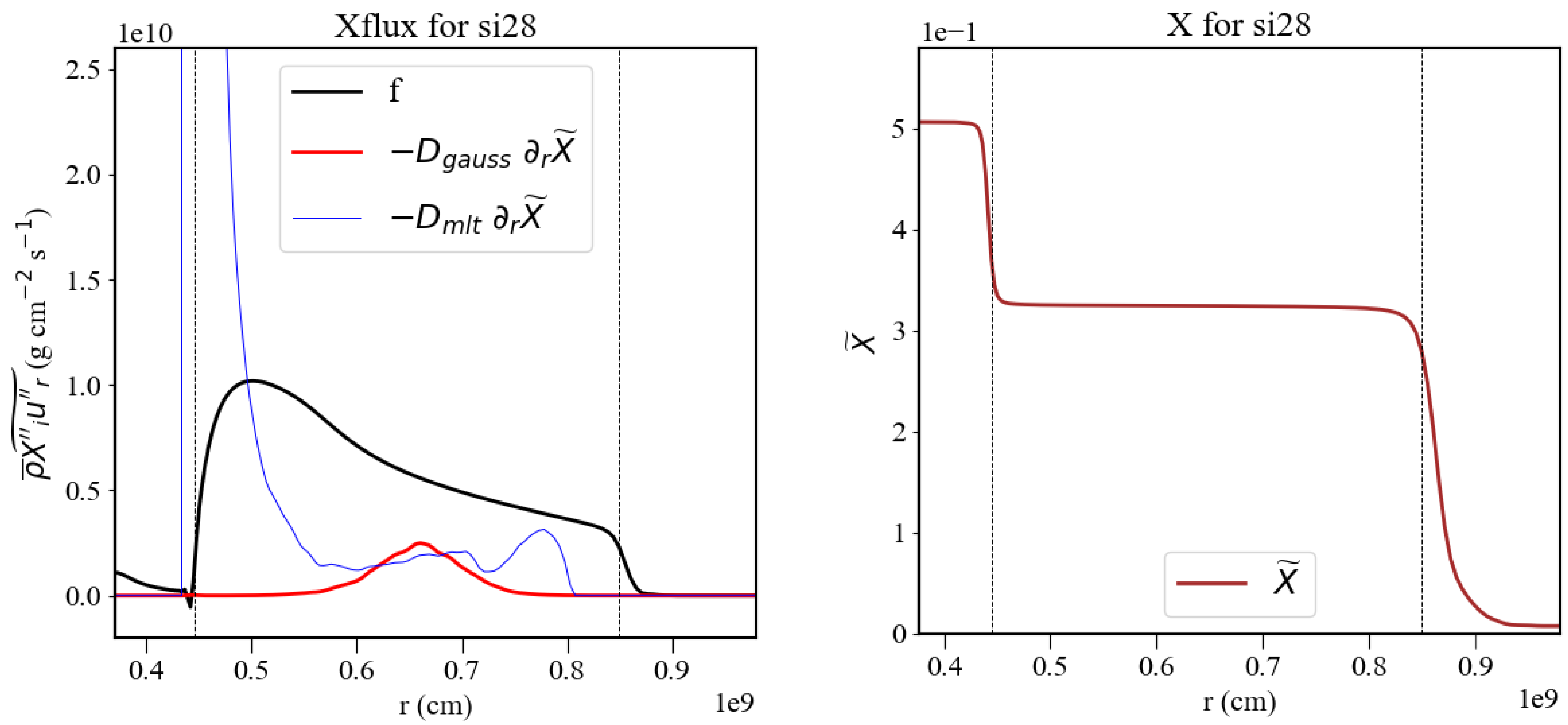




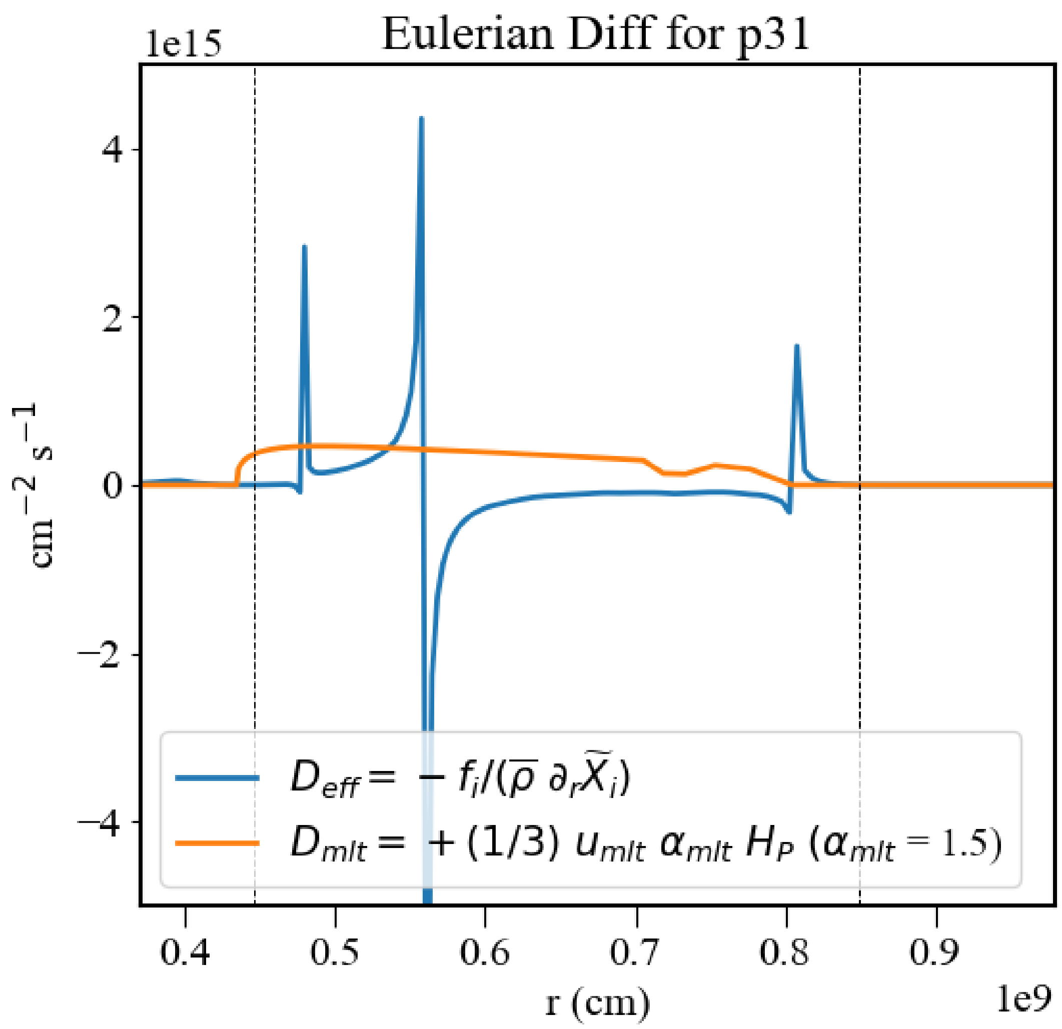
Composition flux model



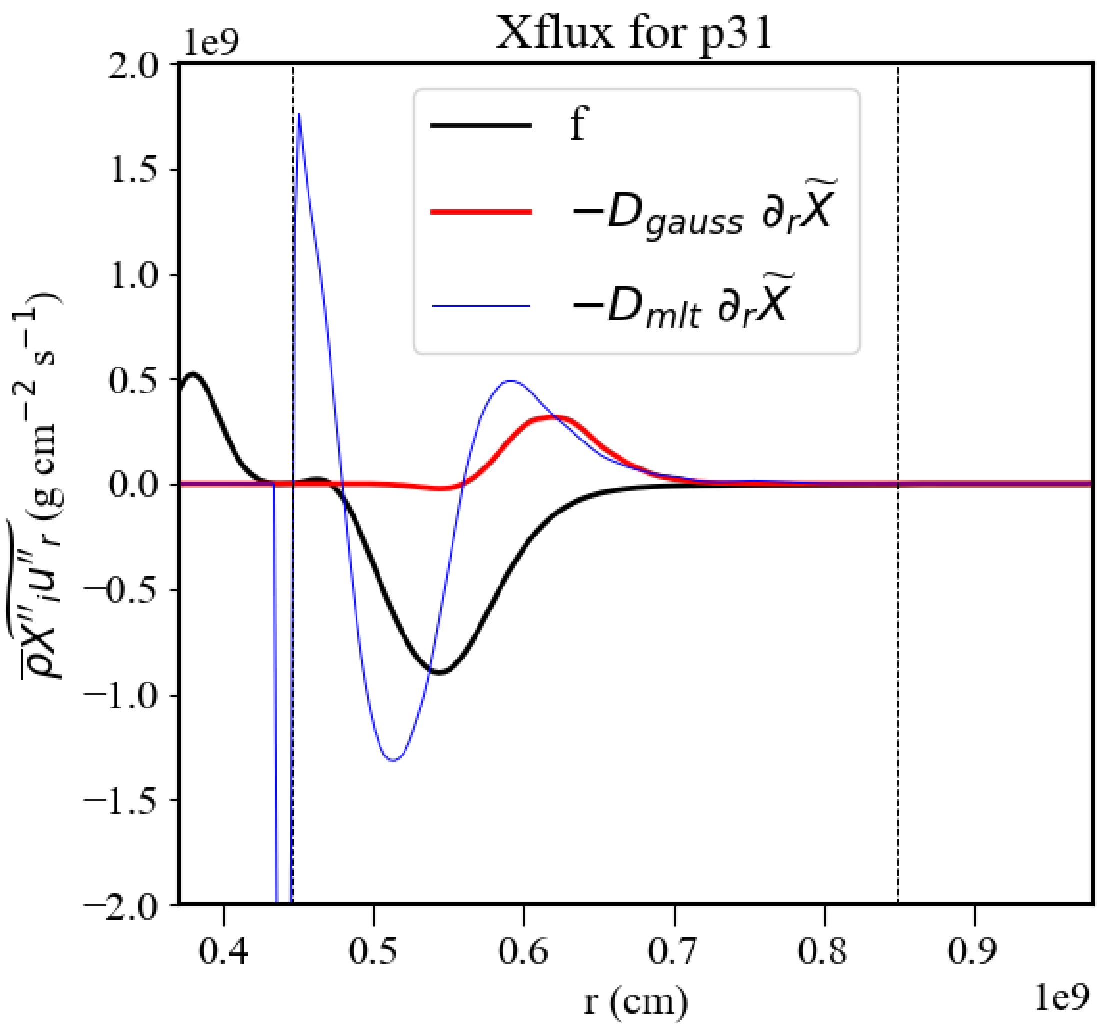
Composition flux model

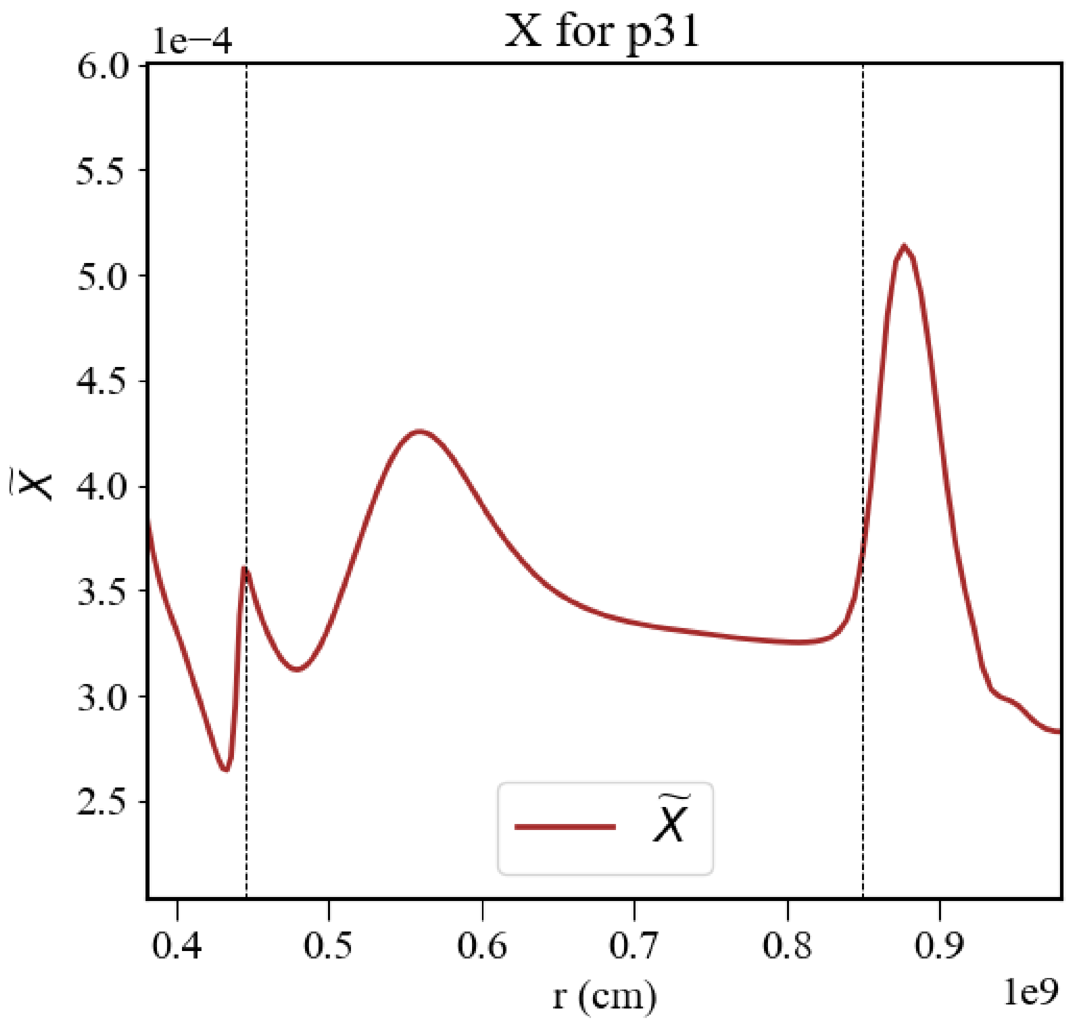


Composition flux model



Composition flux model





Downgradient approximation

$$\widetilde{F}_i^q \sim -\Gamma_t \frac{\partial \widetilde{q}}{\partial x_i} \quad (\Gamma_t \text{ is turbulence diffusivity and } \widetilde{F}_i^q = \overline{\rho q'' u_i''} \text{ is a flux of } q)$$

- can be derived from a transport equation of a diffusive passive scalar (Harlow & Hirt, 1969; Daly & Harlow, 1970):

$$\partial_t \widetilde{F}_i^q - \overline{u_i'' q'' \partial_t \rho} - \widetilde{R}_{in}\partial_n \widetilde{q} + \widetilde{u}_n \rho \partial_n \overline{u_i'' q''} + \widetilde{F}_n^q \partial_n \widetilde{u}_i + \partial_n \overline{\rho u_n'' u_i'' q''} - \overline{u_i'' q'' \partial_n \rho u_n''} = -\overline{q''}\partial_i \overline{P} - \overline{q'' \partial_i P'} + \partial_n(\overline{\lambda \rho u_i'' \partial_n q''}) + f \widetilde{F}_i^q$$

where q is the passive scalar governed by a diffusion equation $D_t q = \lambda \nabla^2 q$

It implies, that the downgradient approximation holds only for:

- a transport of a diffusive passive scalar
- a flow in steady state ($\partial_t \widetilde{F}_i^q = 0$)
- an incompressible flow ($\partial_t \rho = 0$)
- a flow with no background velocities ($\widetilde{u}_i = 0$)
- a flow with no pressure-scalar correlations ($\overline{q''}\partial_i \overline{P} = \overline{q'' \partial_i P'} = 0$)
- a homogeneous flow ($\partial_n \overline{\rho u_n'' u_i'' q''} = 0$)
- an isotropic flow (decay-rate assumption: $\overline{\partial_n q'' \partial_n \rho u_i''} \sim f \widetilde{F}_i^q$)

But, stellar turbulent convection is:

- stratified (not homogeneous)
- anisotropic
- compressible on expanding/contracting background

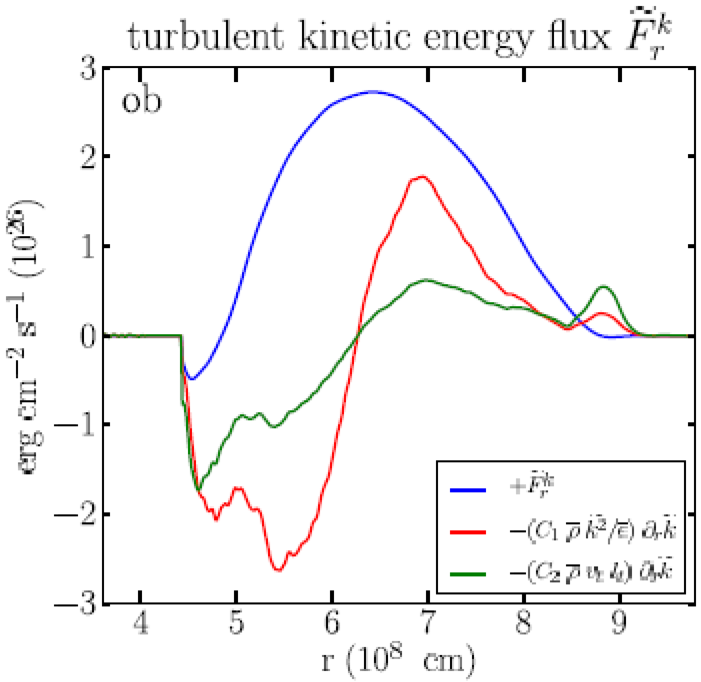


Figure 1: Downgradient approximations to the turbulent kinetic energy flux $\widetilde{F}_r^k = \overline{\rho u_r'' k''}$ derived from 3D oxygen burning shell model.

– **downgradient approximation is not suitable for modelling stellar processes**