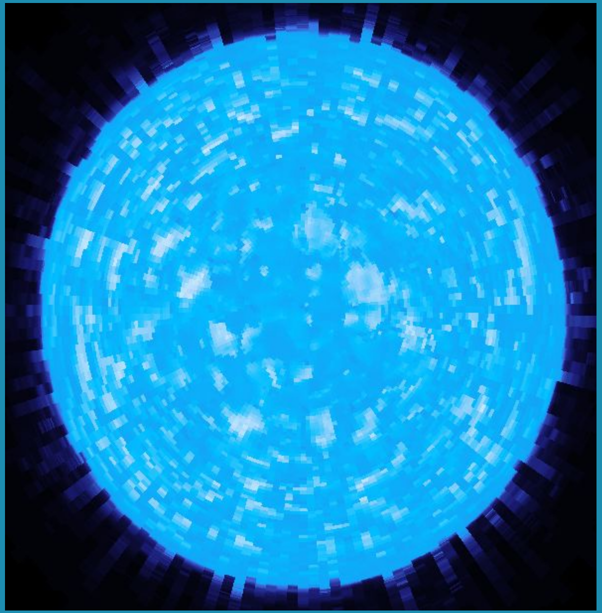
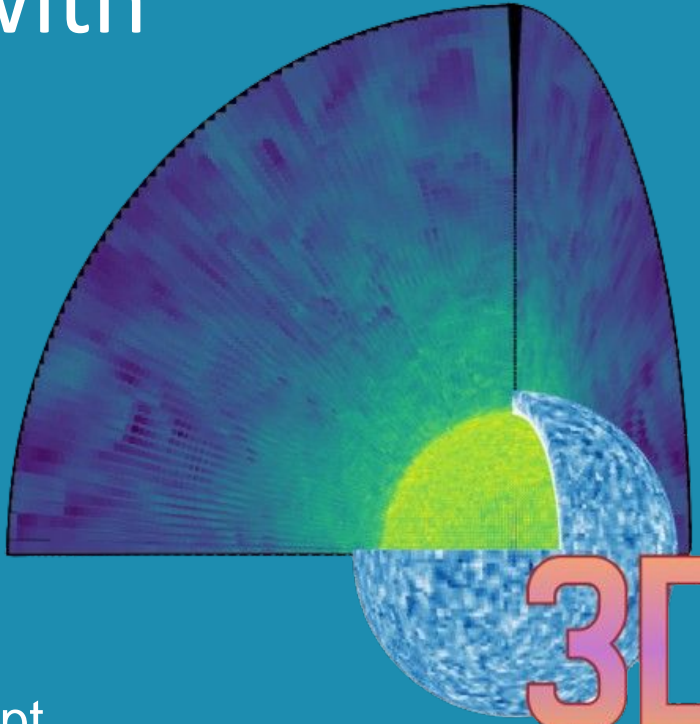


Toward spectral analysis with 3D model atmospheres

Lara Delbroek

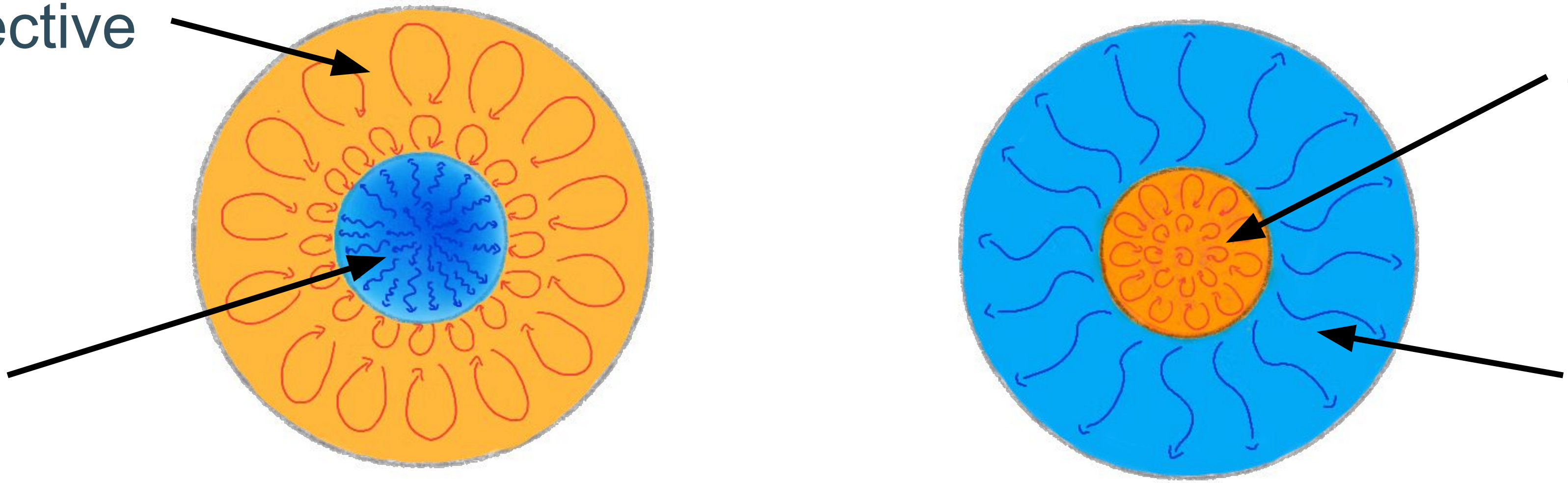
& 'SUPERSTARS-3D' team:

Jon Sundqvist	Nicolas Moens
Luka Poniatowski	Frank Backs
Olivier Verhamme	Cassandra Van der Sijpt
Dwaipayan Debnath	Pieter Schillemans



Why 3D radiative transfer techniques/models?

Classical view:



Low Mass

Convective

Radiative

High Mass

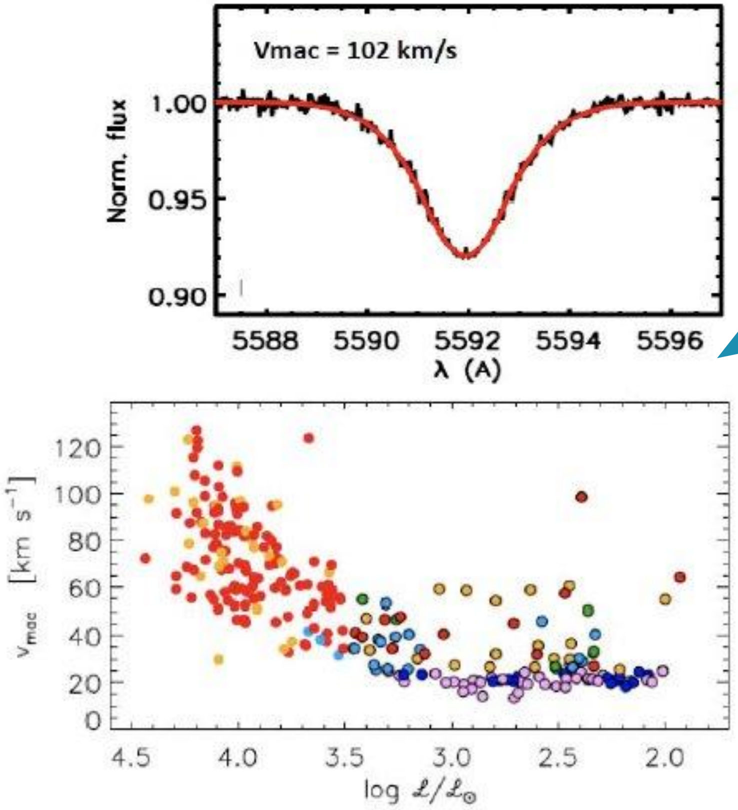
Convective

Radiative

stable (1D) envelopes and atmospheres

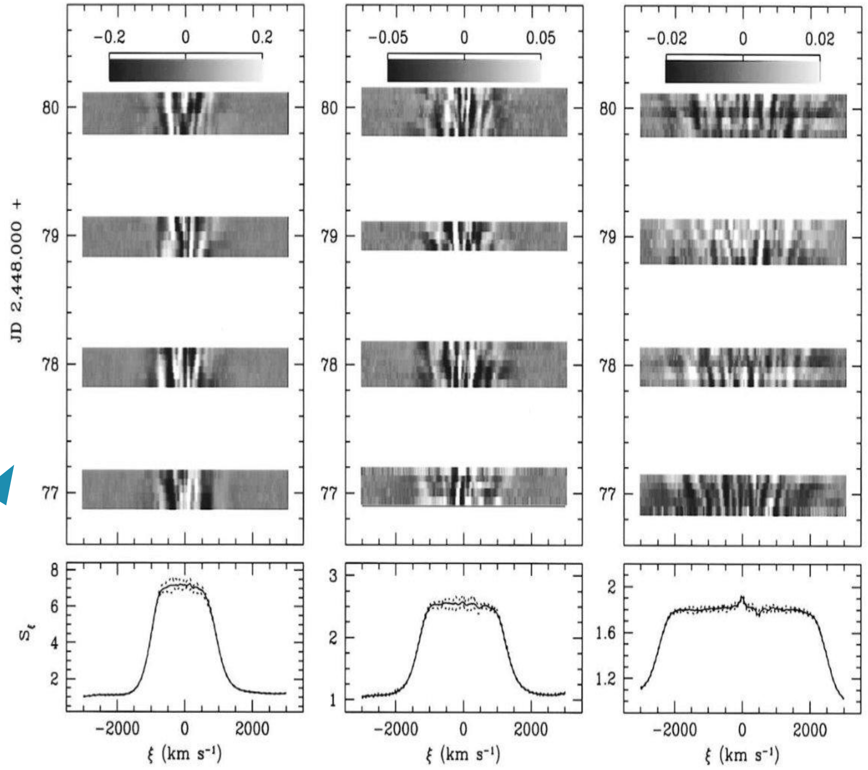
Why 3D radiative transfer techniques/models?

spectroscopic observations: indications for 3D, time-dependent effects



- Optical absorption (photospheric) lines indicate very large (‘micro’ and/or) ‘macroturbulent’ velocities

- Optical emission (wind) lines indicate line-profile variability



Simon-Diaz+ 2014

Lepine & Moffat (1999)

Why 3D radiative transfer techniques/models?

- Higher mass stars: can’t resolve surface (contrast to Sun)

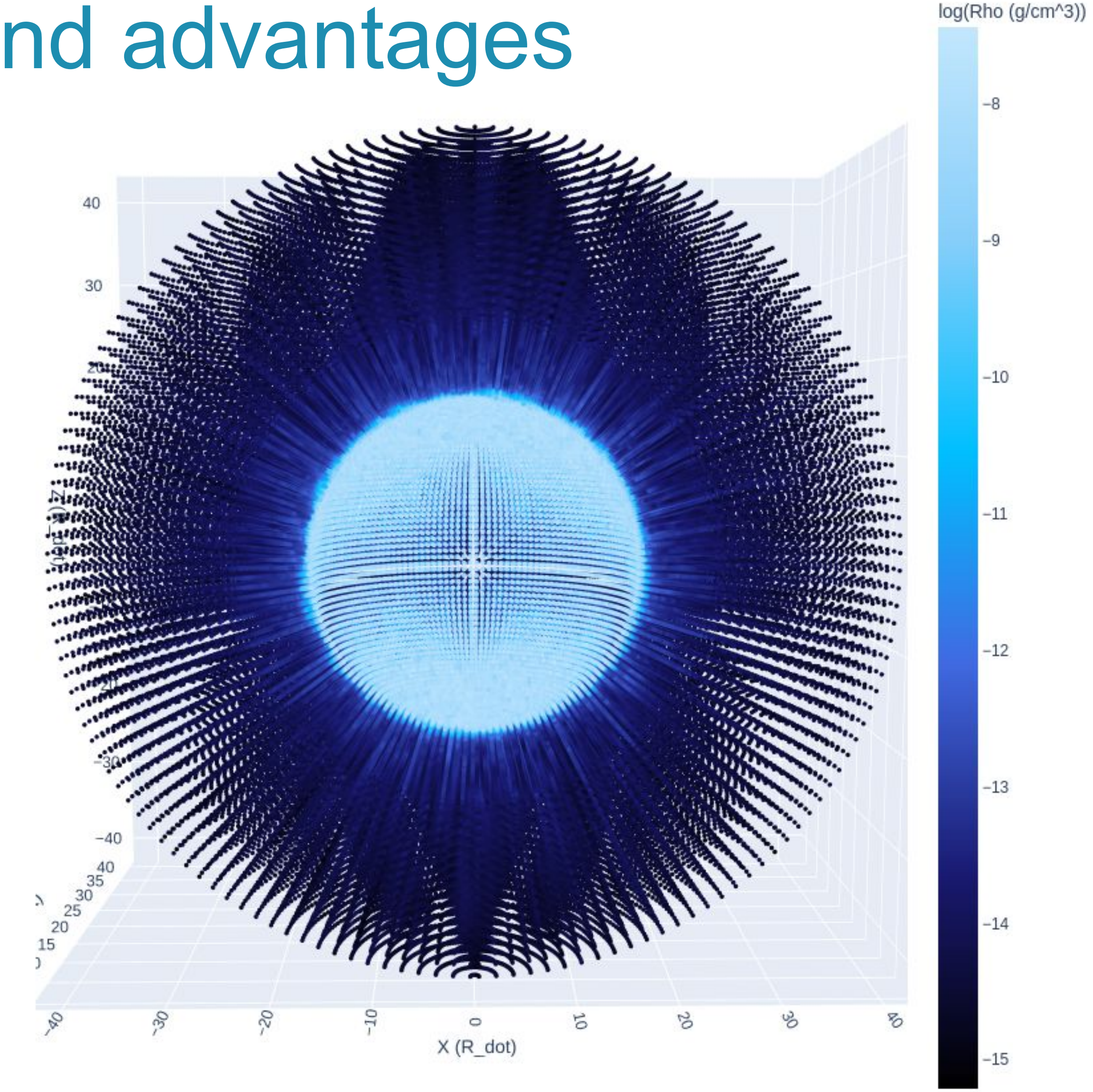
- Need ‘quantitative spectroscopy’ to test models and compare these models with observations

- Post-Processing 3D-RT packages building on Hennicker et al. (2020,2021)

Which techniques and advantages

- 3D radiative transfer techniques (building from Hennicker et al. 2021) applied to the first 3D unified atmosphere and wind simulations of O-type stars.

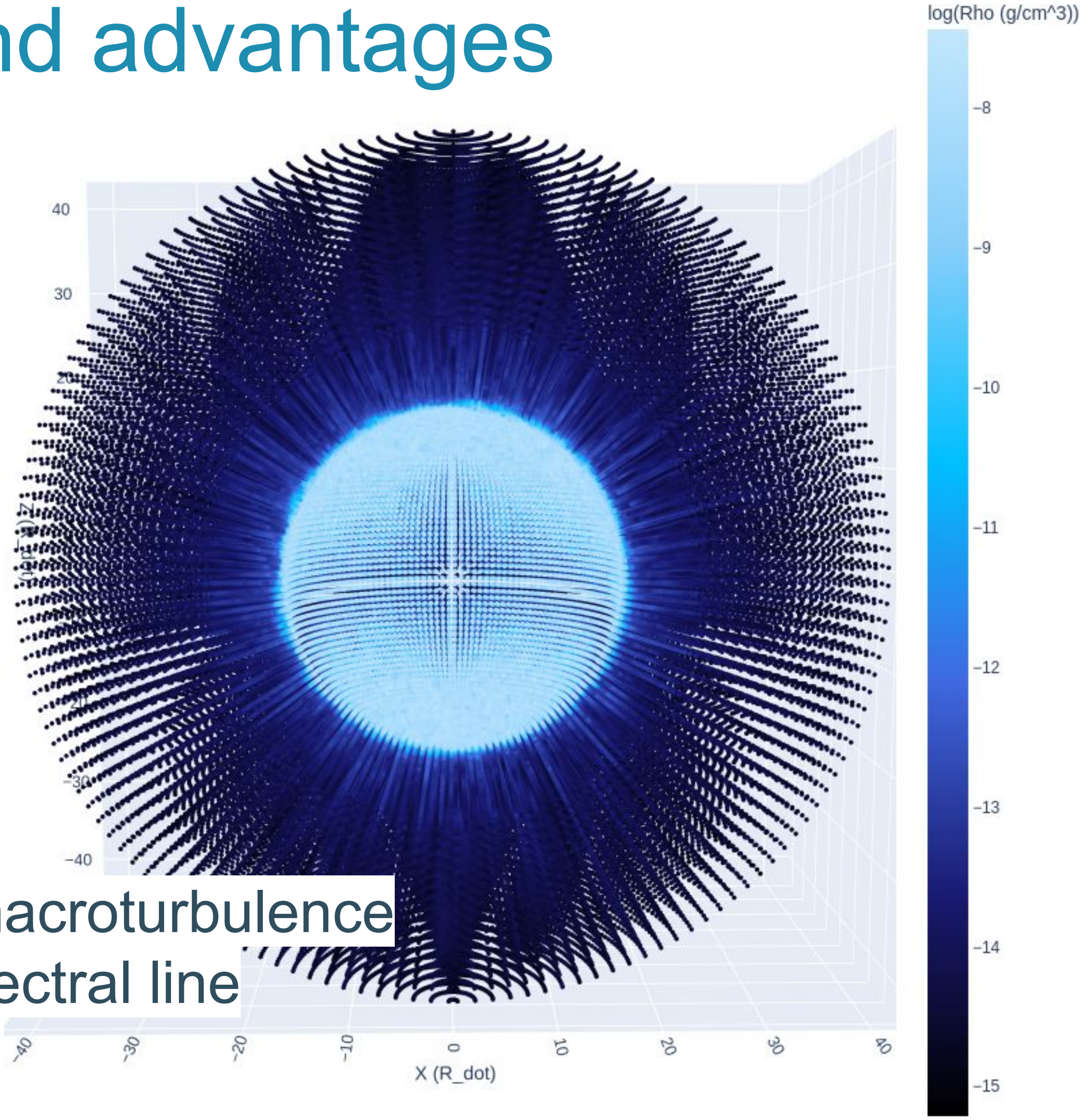
- 3D model: Moving away from 'free parameter heaven/hell'



Which techniques and advantages

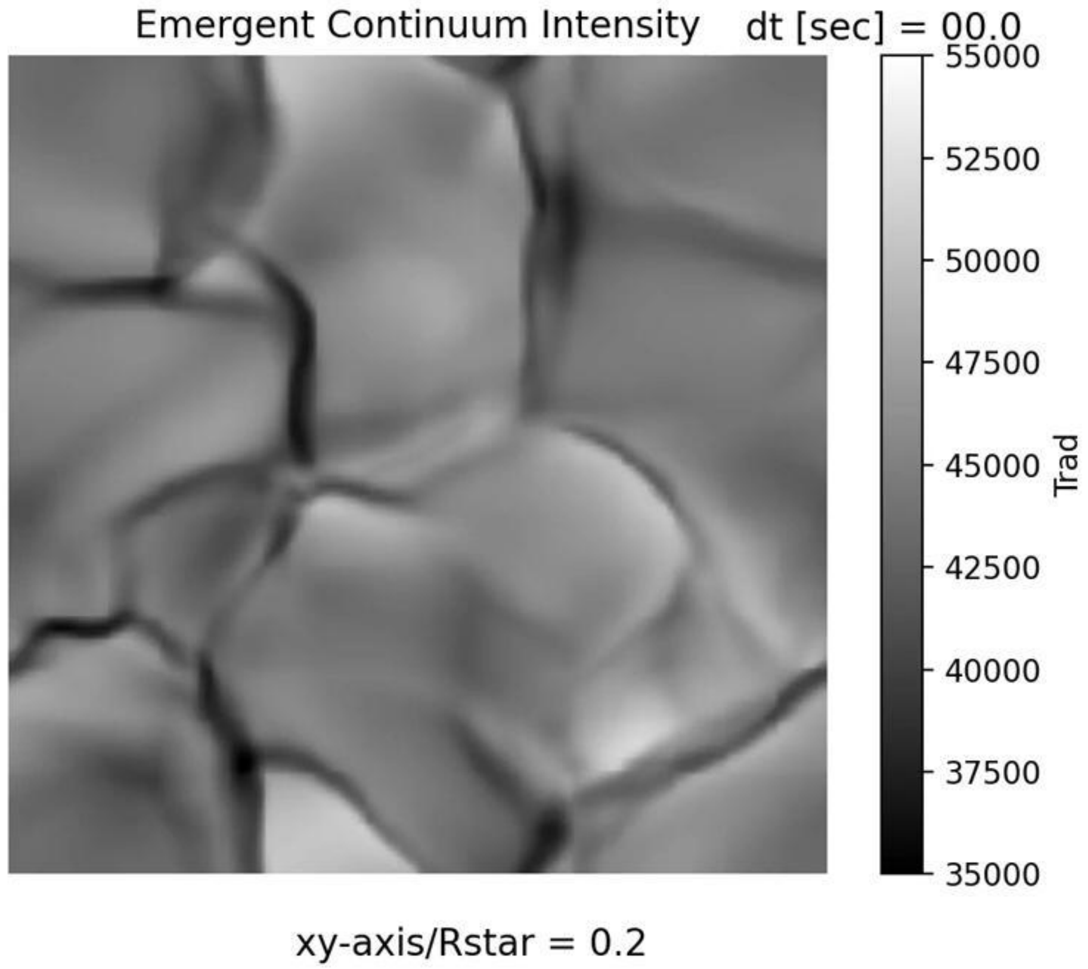
3D model: Moving away from 'free parameter heaven/hell’

1D models		3D models
M	β	M
L	Vmic	L
R	Vmac	R
[Fe/H]	fcl	[Fe/H]
v sin i	fvel	
$\dot{M}$	vcl	
v_∞	…	



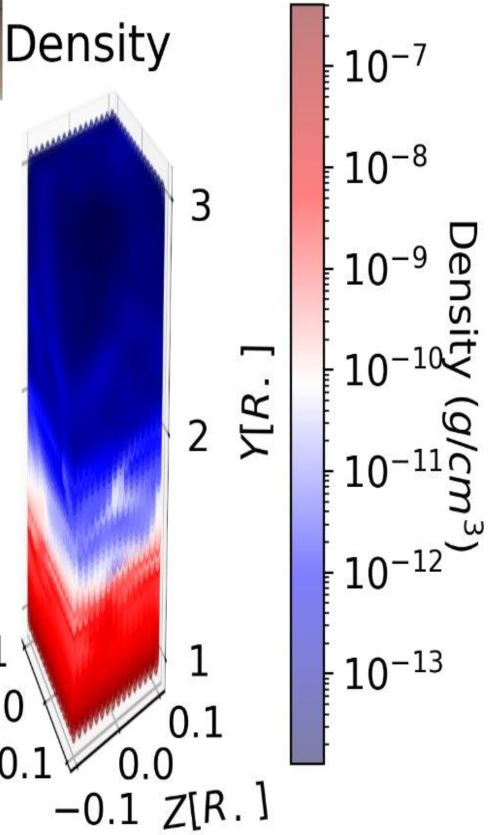
No micro-/macroturbulence added in spectral line formation!

O-star view from orbit



- Emergent intensity (surface brightness) at one frequency point in the optical continuum (LTE)
- HUGE fluctuations across surface in emergent radiation temperature
- We cannot resolve surface of O-stars (contrast to Sun) => Need of flux profiles for full star (not just patch!)
- Transition: 3D box to sphere

Constructing 3D spherical model



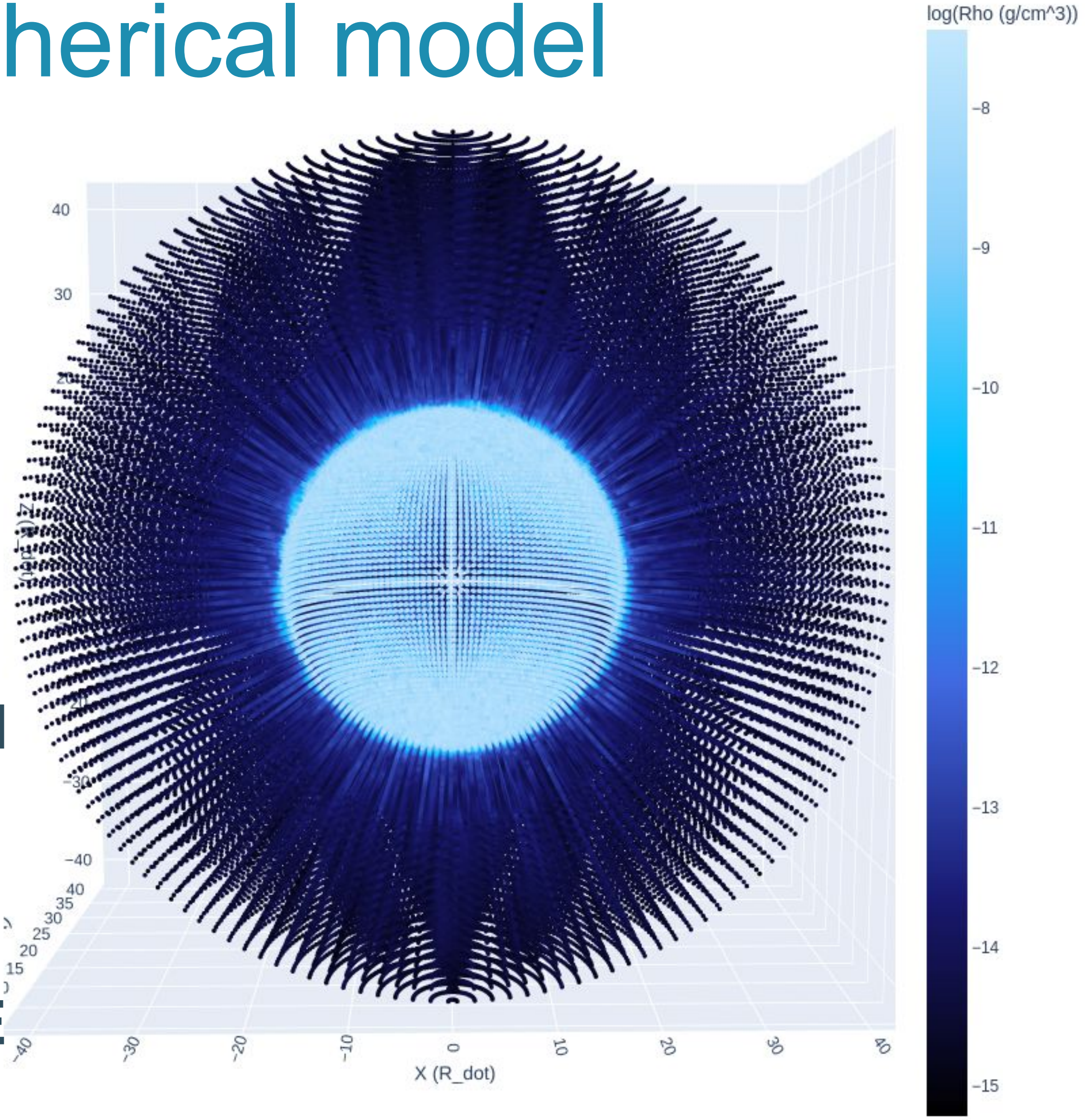
3D O-star models

100 snapshots

Source functions and opacities calculation

2 options:

- LTE
- **approximate NLTE**



Radiative transfer: equations

- Time-independent equation of radiative transfer:

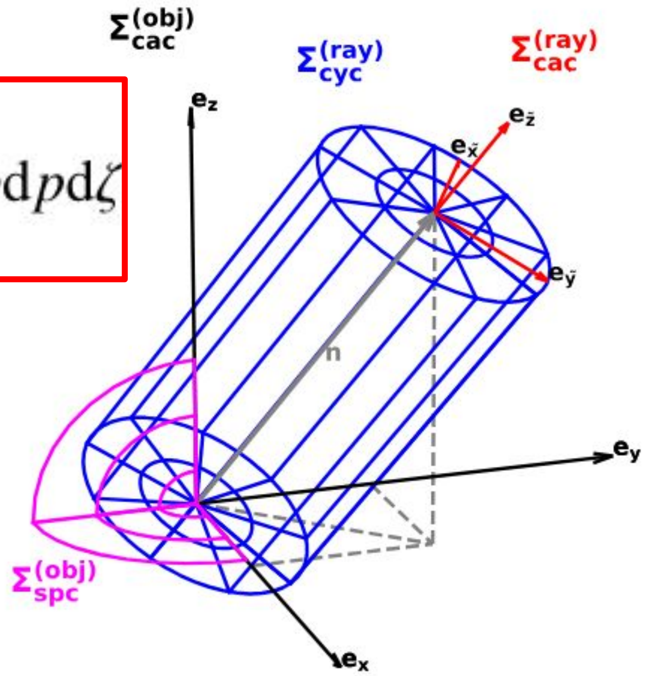
$$\boldsymbol{n}\boldsymbol{\nabla} I_\nu = \eta_\nu - \chi_\nu I_\nu = \chi_\nu (S_\nu - I_\nu)$$

I_ν = specific intensity ; η_ν = emissivity ; χ_ν = opacity ; $S_\nu = \eta_\nu/\chi_\nu$ = source function

- Emergent flux profiles:

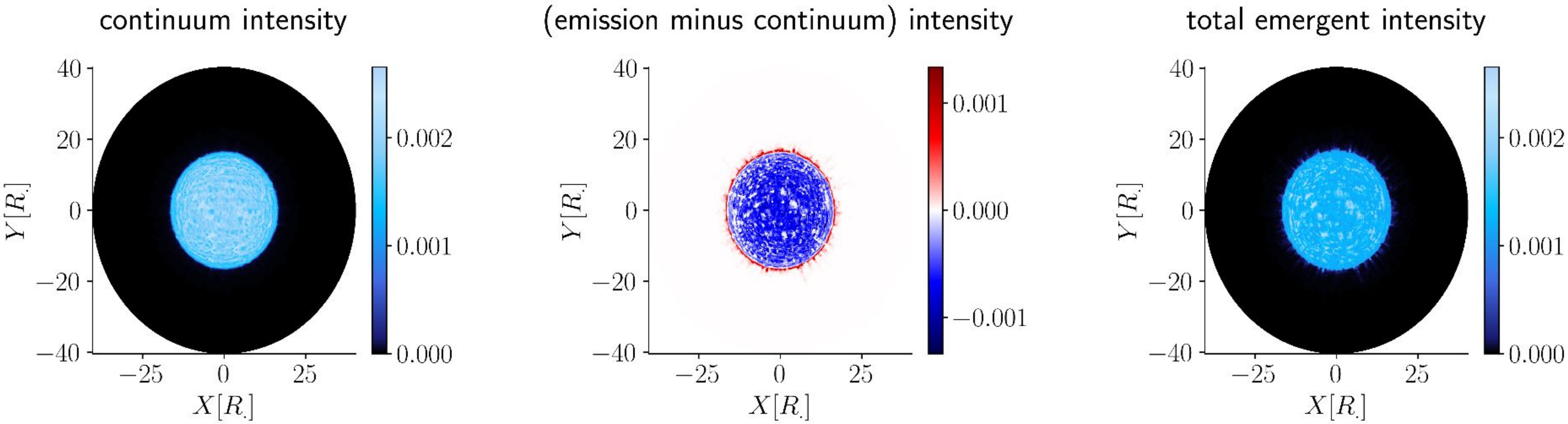
$$F_\nu = \frac{1}{d^2} \int_0^{2\pi} \int_0^{R_{\max}} I_\nu (p, \zeta, \tilde{z} = R_{\max})\, p \mathrm{d}p \mathrm{d}\zeta$$

- specific intensity I_ν used for surface brightness (pz geometry)



Hennicker et al 2022

Surface brightness/emergent flux profiles


continuum intensity

(emission minus continuum) intensity

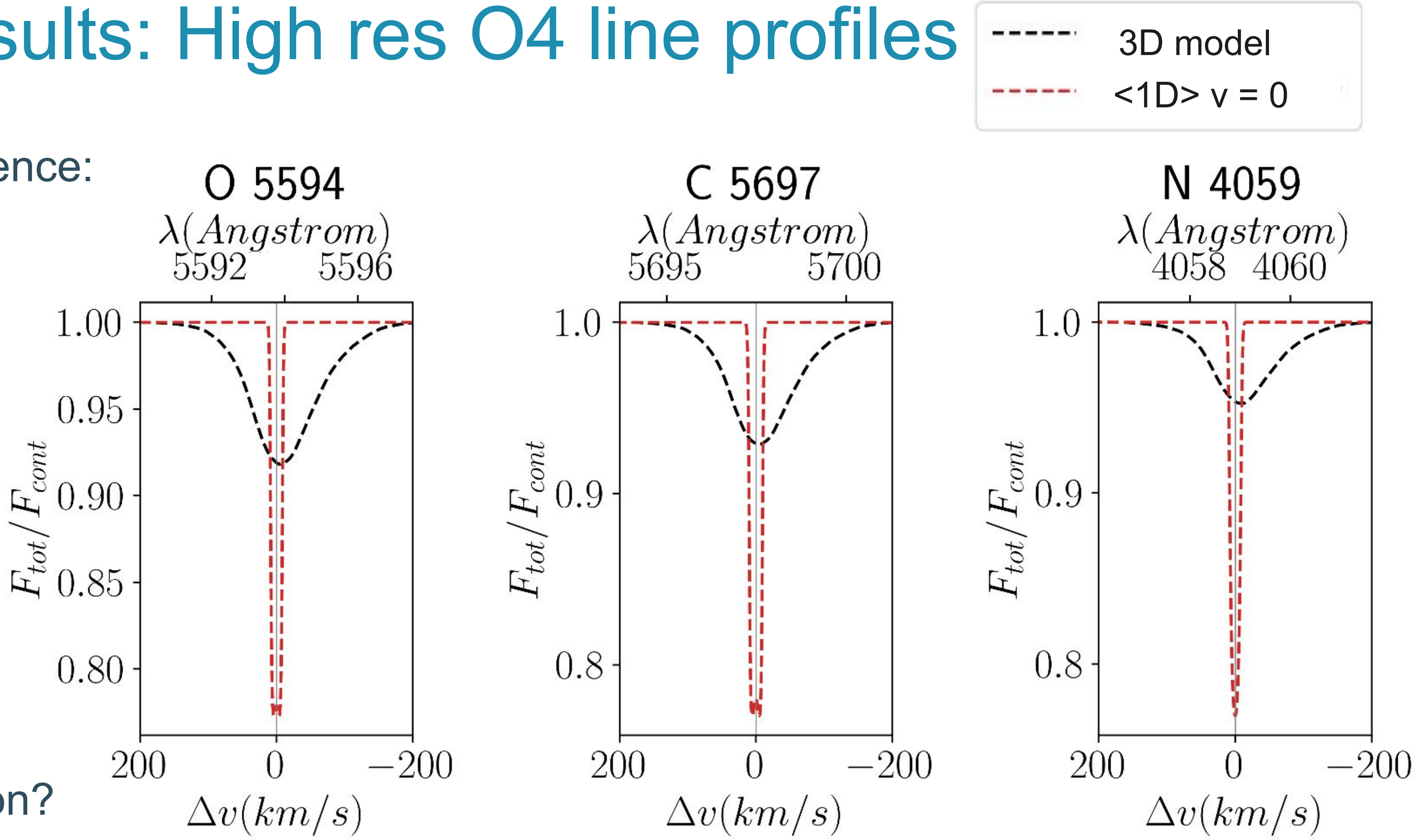
total emergent intensity

At an average $\langle\tau_r\rangle = \frac{2}{3}$:

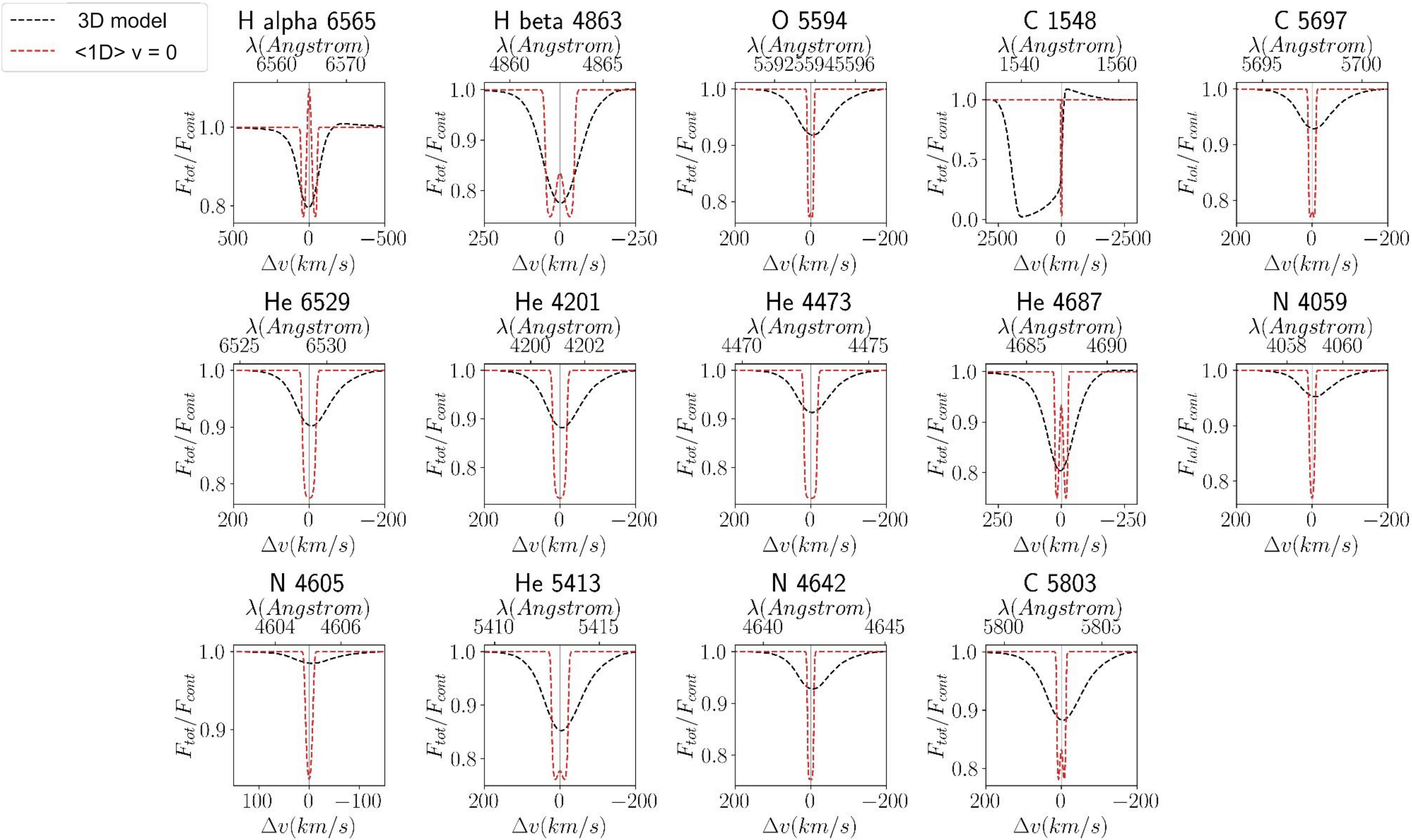
Temperature	38 kK
Mstar_Msun	58.3
Rstar/Rsun	16.3
log g star	3.78
Mass loss	1e-6 solar mass/year

Results: High res O4 line profiles

- No micro/macro- turbulence:
  => natural explanation
  ‘extra broadening’
  observed in O-stars
- v = 0 lines very narrow
  => need extra ad-hoc
  broadening 1D model
  atmosphere codes
- EW (3D) > EW (v = 0)
  1D codes for
  spectropscopy:
  3D abundance correction?
  microturbulence?
  To be explored



KU LEUVEN



3D model
<1D> v = 0
H alpha 6565
H beta 4863
O 5594
C 1548
C 5697
He 6529
He 4201
He 4473
He 4687
N 4059
N 4605
He 5413
N 4642
C 5803
$\lambda(Angstrom)$
6560
6570
4860
4865
559255945596
1540
1560
5695
5700
6525
6530
4200
4202
4470
4475
4685
4690
4058
4060
4604
4606
5410
5415
4640
4645
5800
5805
F_{tot}/F_{cont}
1.0
0.9
0.8
0.5
0.0
$\Delta v(km/s)$
500
0
−500
250
−250
200
−200
2500
−2500
100
−100

Summary

- 3D-RT package to explore effects on spectra (Multi-D O-star atmosphere with wind models)
- Very turbulent atmosphere, large velocity fields and density variations also in photosphere
- Unlike 1D-atmosphere codes no micro- or macroturbulence needed
- Observed (high-resolution, high S/N) line widths, shapes, and shifts might be used as critical tests
- Relative 3D effects on chemical abundance and stellar parameter derivation to be explored (See also talk by Gemma Gonzalez)

Supplementary slides

Radiative transfer: equations

- Time-independent equation of radiative transfer:

$$\boldsymbol{n}\nabla I_\nu = \eta_\nu - \chi_\nu I_\nu = \chi_\nu (S_\nu - I_\nu)$$

I_ν = specific intensity ; η_ν = emissivity ; χ_ν = opacity ; $S_\nu = \eta_\nu / \chi_\nu$ = source function

- angular moments of the specific intensity :

J_ν = mean intensity ; H_ν = Eddington flux
K_ν = 2nd moment ; P_ν = radiation pressure
F_ν = flux ; E_ν = energy density

$$\begin{aligned}
J_\nu &= \frac{1}{4\pi}\int I_\nu \mathrm{d}\Omega = \frac{c}{4\pi} E_\nu\,, \\
\boldsymbol{H}_\nu &= \frac{1}{4\pi}\int I_\nu \boldsymbol{n} \mathrm{d}\Omega = \frac{1}{4\pi} \boldsymbol{F}_\nu\,, \\
\boldsymbol{K}_\nu &= \frac{1}{4\pi}\int \underbrace{\boldsymbol{n} I_\nu \boldsymbol{n}}_{\text{dyadic product}} \mathrm{d}\Omega = \frac{c}{4\pi} \boldsymbol{P}_\nu\,,
\end{aligned}$$

Radiative transfer: equations

Solve radiative transfer (in a pz-type geometry) to obtain surface brightnesses/ emergent flux profiles

- To get emergent intensity: formal integral
  - Get emergent intensity at each point on surface for each frequency: solve RT equation
  - For this you need: opacities AND source functions at all spatial points
  - Assumption: opacities (line and continuum) and source functions can be calculated locally for a given 3D structure (temperature, velocity, density)

- To get emergent flux: angle integration over projected surface

Post-Processing 3D-RT packages building from Hennicker et al. (2020,2021)
Line opacity method: Poniatowski et. (2022)

Radiative transfer: equations

- Assumptions LTE: opacities via Saha-Boltzmann relations and source functions via planck function
- Assumptions aNLTE: it approximates NLTE deviations from LTE by a local approach, it modifies the Saha-Boltzmann relations when computing number densities (refs, Lucy & Abbott 1993, Springmann & Puls, ‘fastwind’)
- For full NLTE (NOT IN USE YET, much more time consuming):
  source functions DEPEND on J_ν (zero angular moment). Need to solve RT equation for I_ν and angular moment to get J_ν for ALL points in atmosphere. THEN with this new J_ν update values for S_ν, repeat process. Done until S_ν converged: Lambda iteration (accelerated technique: accelerated lambda iteration (ALI)). Built in for a source function containing scattering.

Post-Processing 3D-RT packages building from Hennicker et al. (2020,2021)
Line opacity method: Poniatowski et. (2022)

Modelspec:

LTE vs aNLTE

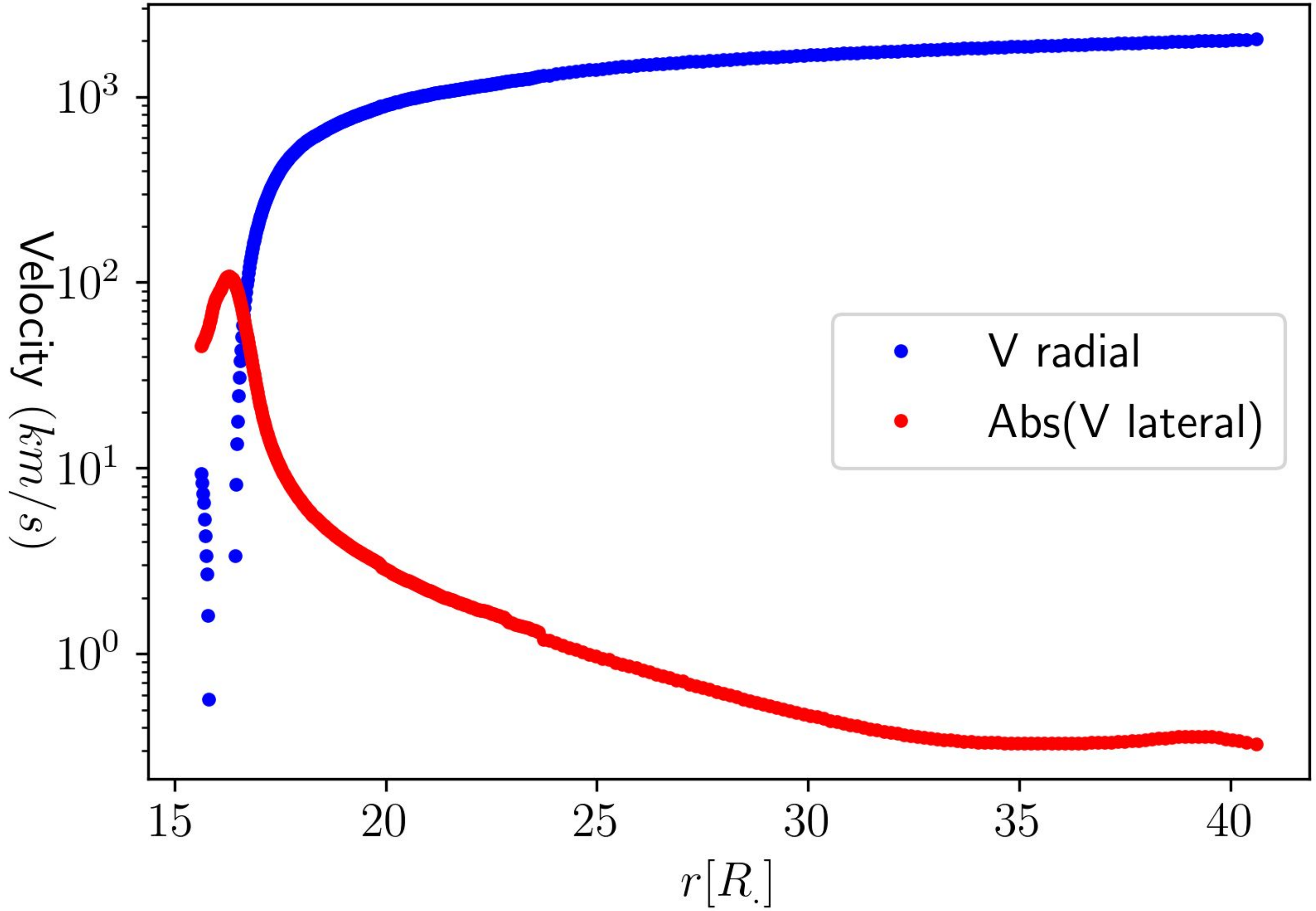
LTE

- Continuum opacity:
  Use Thomson scattering opacity
- Line opacities: LTE
  (LTE opacity package by Poniatowski et. (2022))
- Continuum source function:
  Planck function
- Line source function:
  Planck function

aNLTE

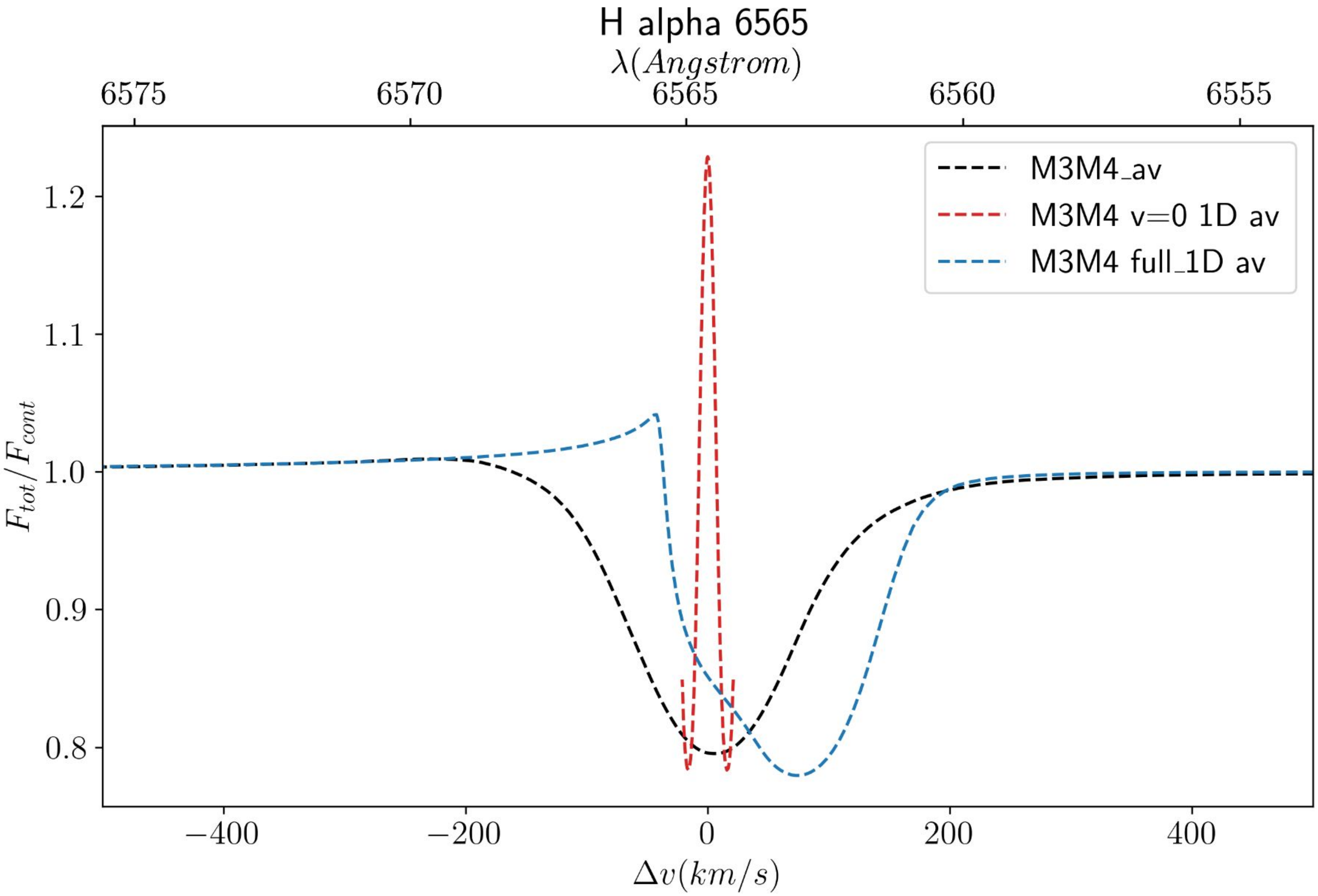
- Continuum opacity:
  Use Thomson scattering opacity
- Line opacities: aNLTE (modifies the Saha-Boltzmann relations when computing number densities), (updated from LTE opacity package by Poniatowski et. (2022))
- Continuum source function:
  Planck function (T_rad)
- Line source function: Planck function with aNLTE modifications

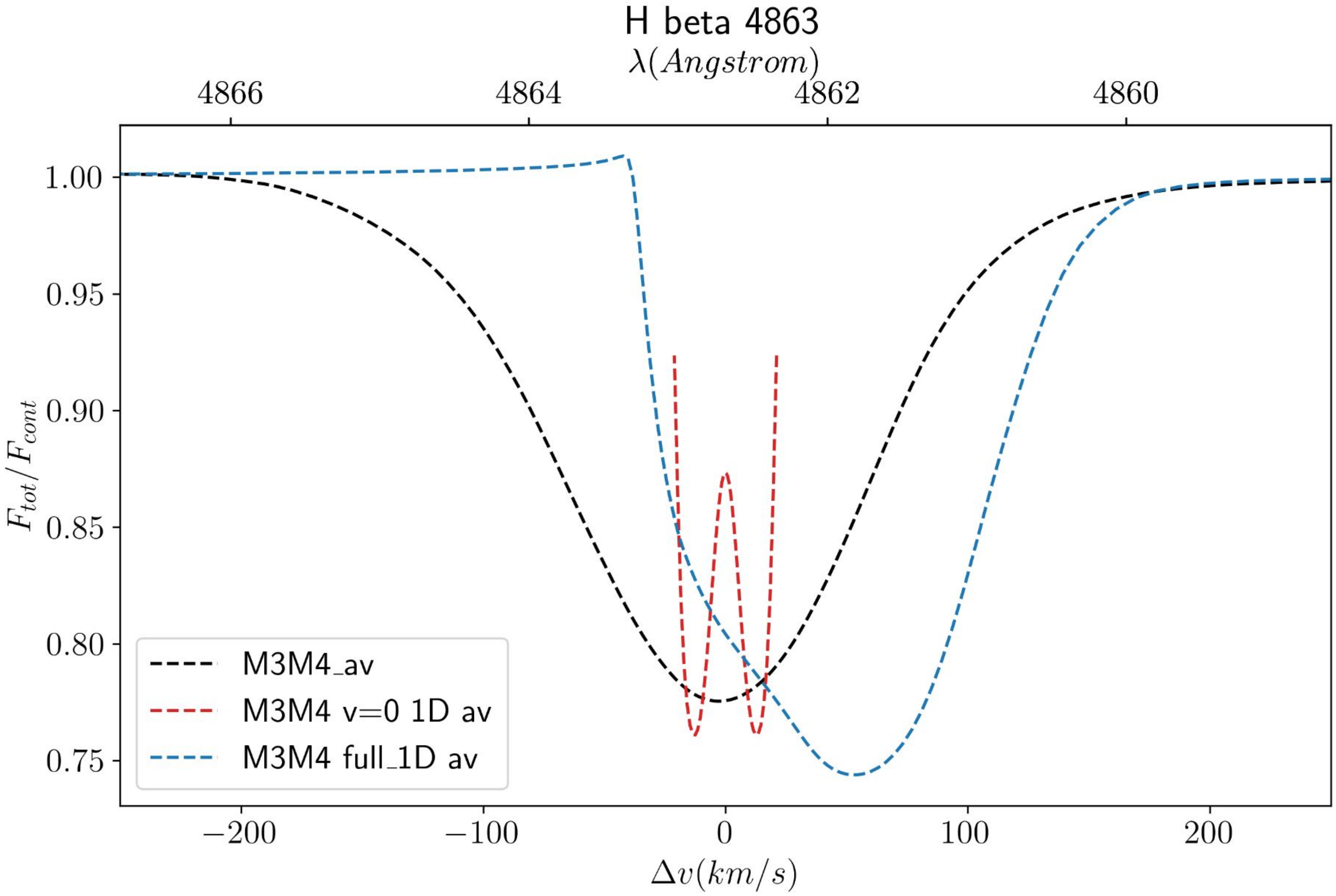
Model 3 Average velocities

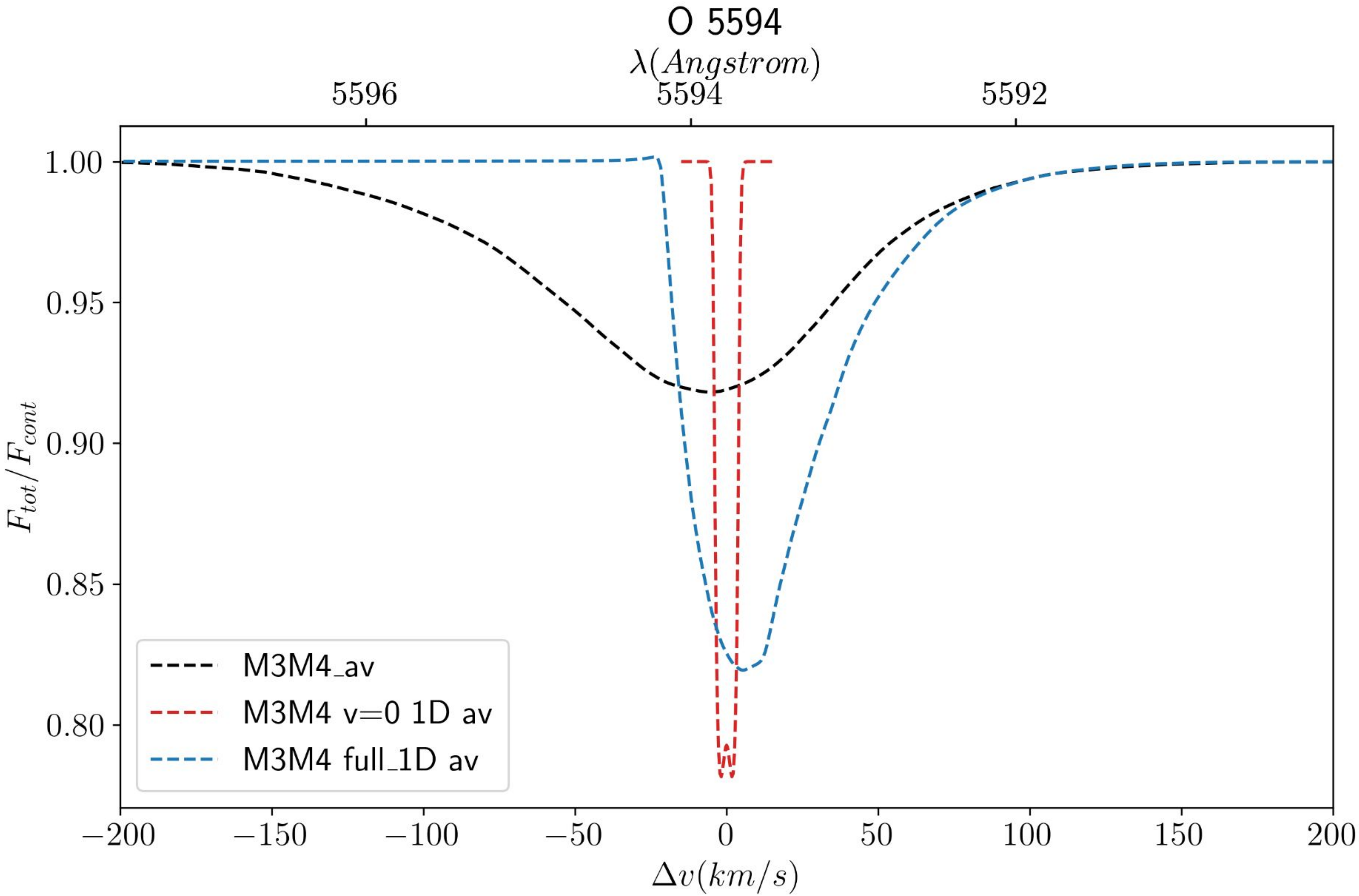


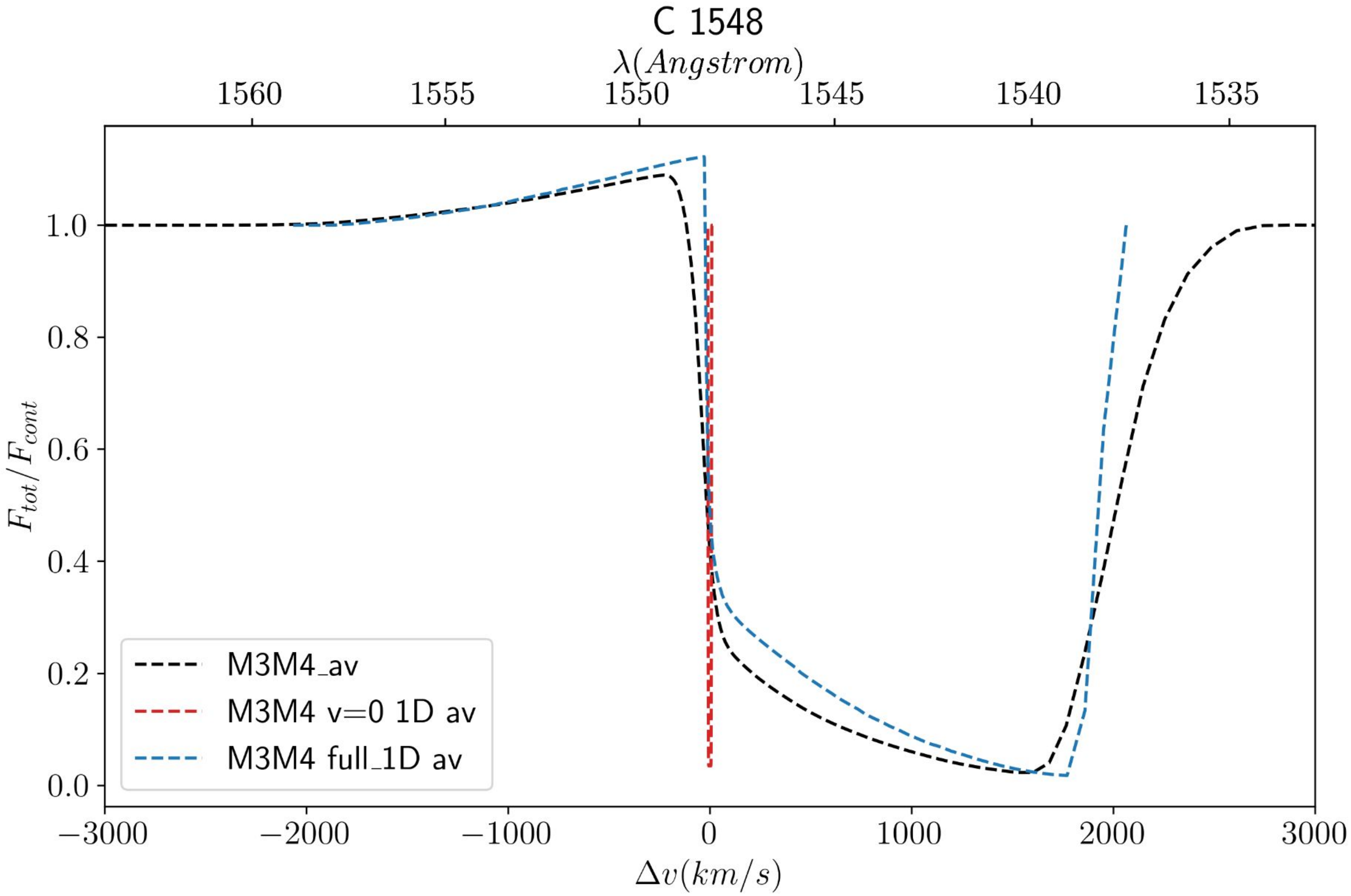
V = 0 averaged in modelspec

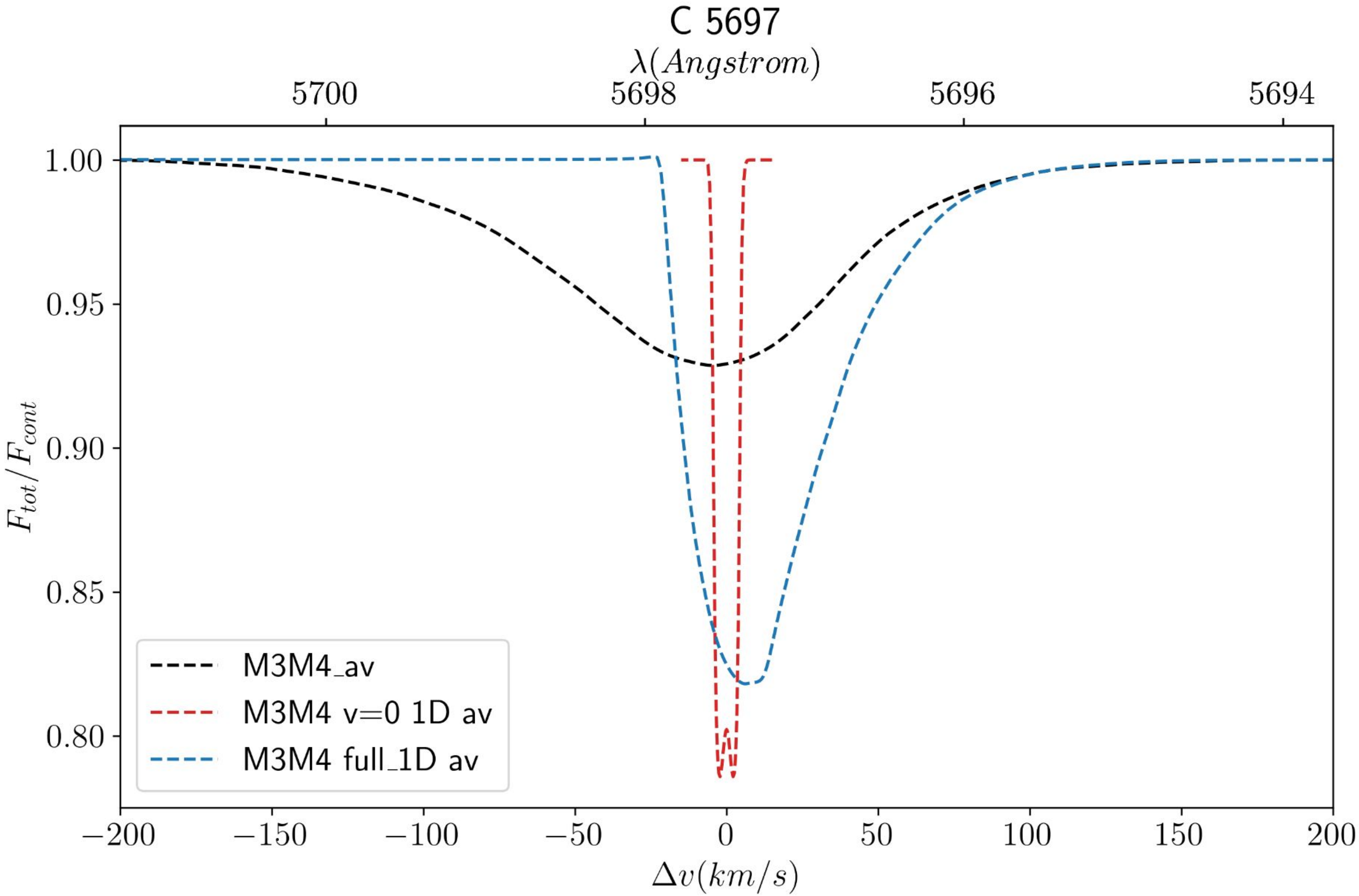
V = v_av averaged in modelspec

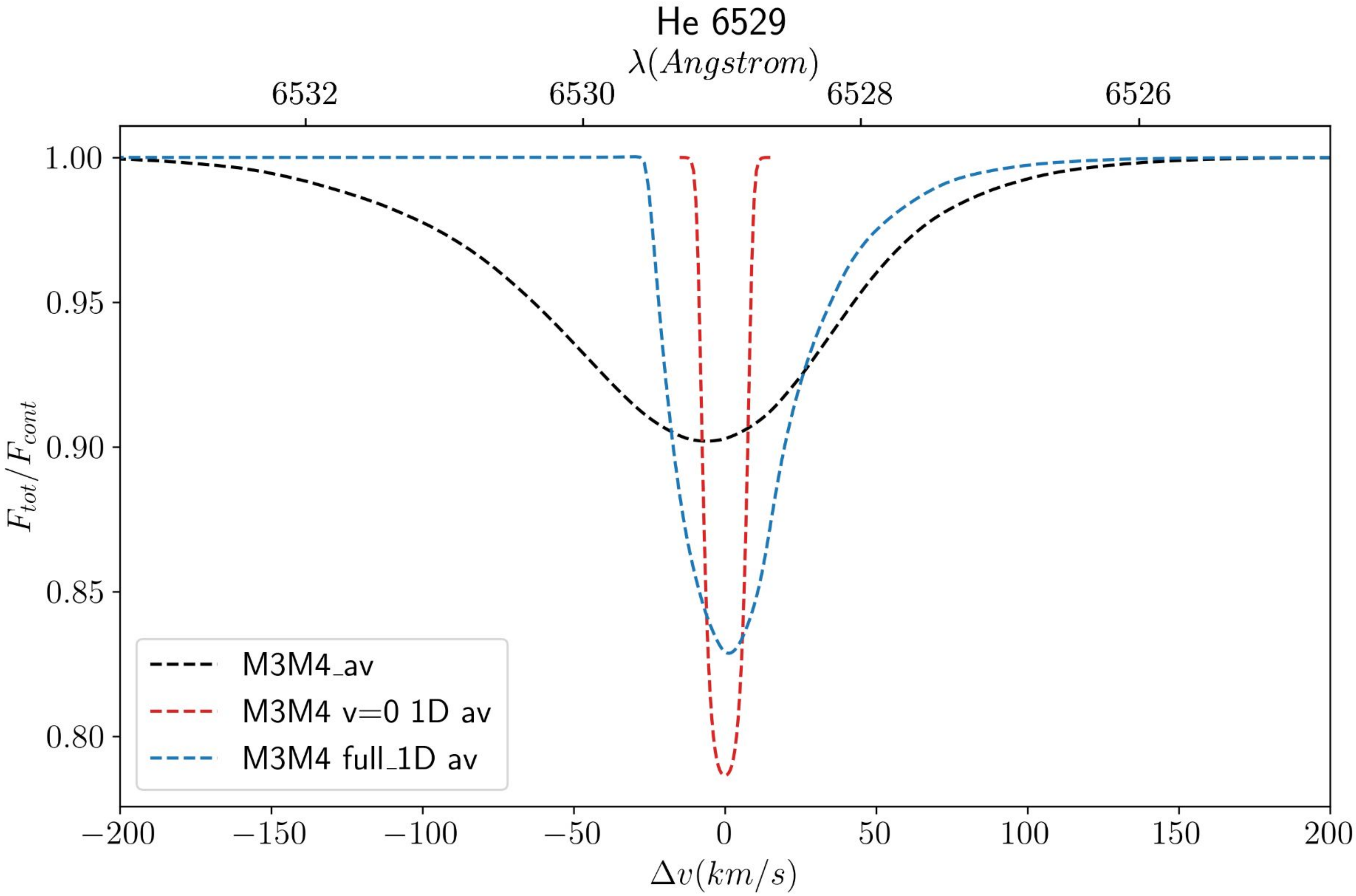

H alpha 6565
$\lambda(Angstrom)$
6575
6570
6565
6560
6555
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
1.2
1.1
1.0
0.9
0.8
F_{tot}/F_{cont}
−400
−200
0
200
400
$\Delta v(km/s)$

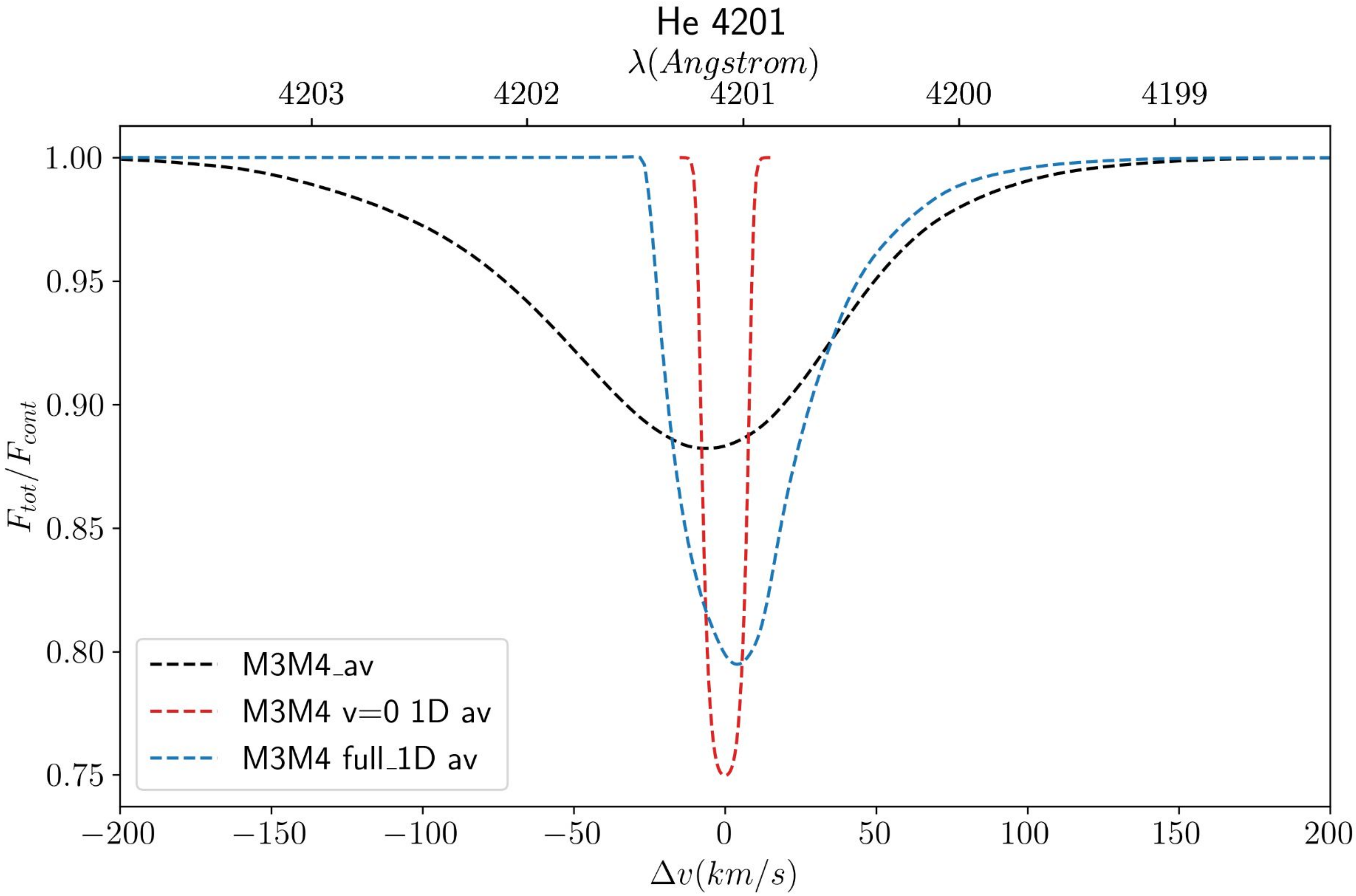

H beta 4863
$\lambda(Angstrom)$
4866
4864
4862
4860
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
0.75
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−100
0
100
200
$\Delta v(km/s)$

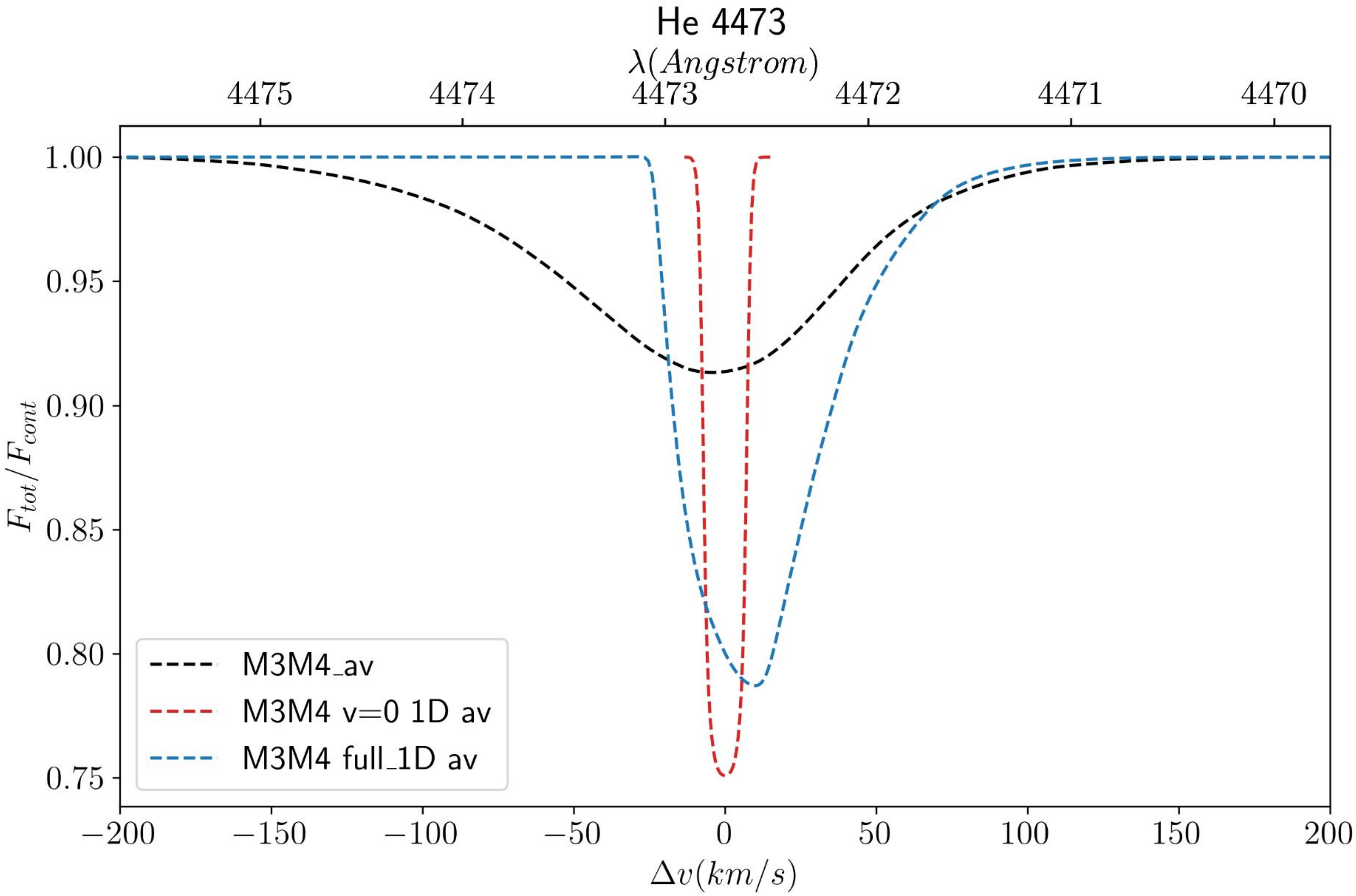

O 5594
$\lambda(Angstrom)$
5596
5594
5592
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
-200
-150
-100
-50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av

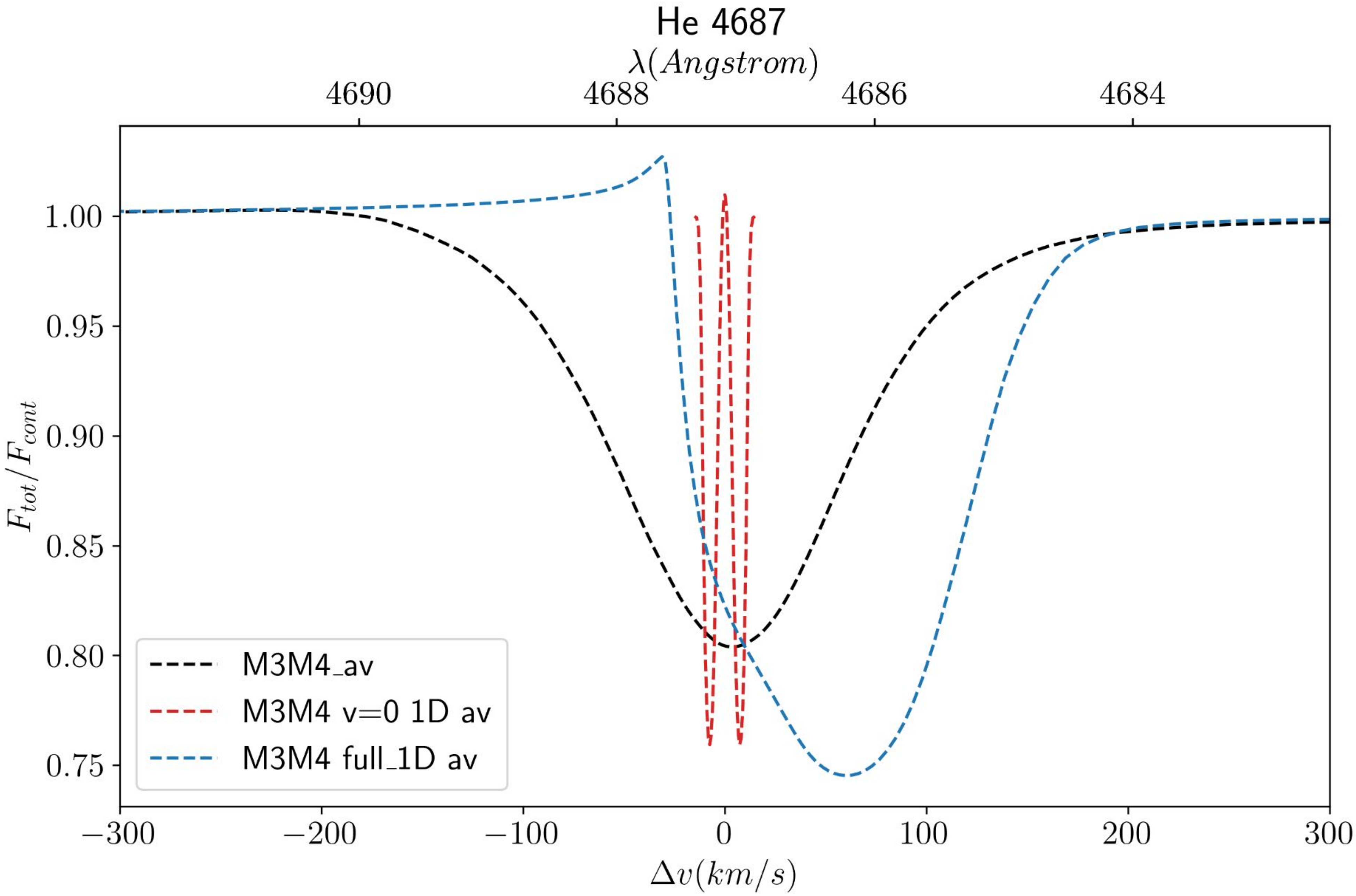

C 1548
λ(Angstrom)
1560
1555
1550
1545
1540
1535
F_{tot}/F_{cont}
1.0
0.8
0.6
0.4
0.2
0.0
−3000
−2000
−1000
0
1000
2000
3000
Δv(km/s)
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av

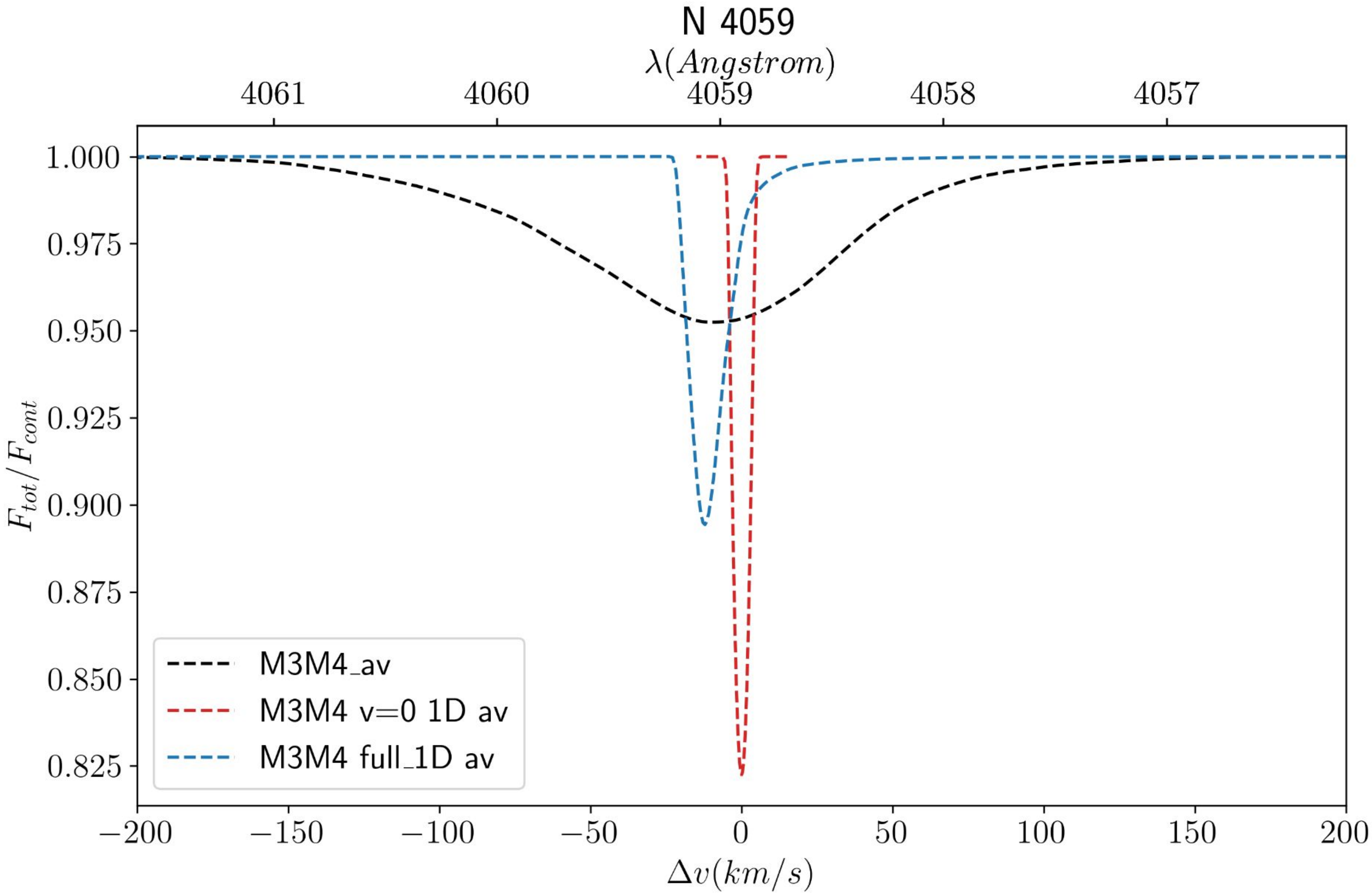

C 5697
$\lambda(Angstrom)$
5700
5698
5696
5694
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$

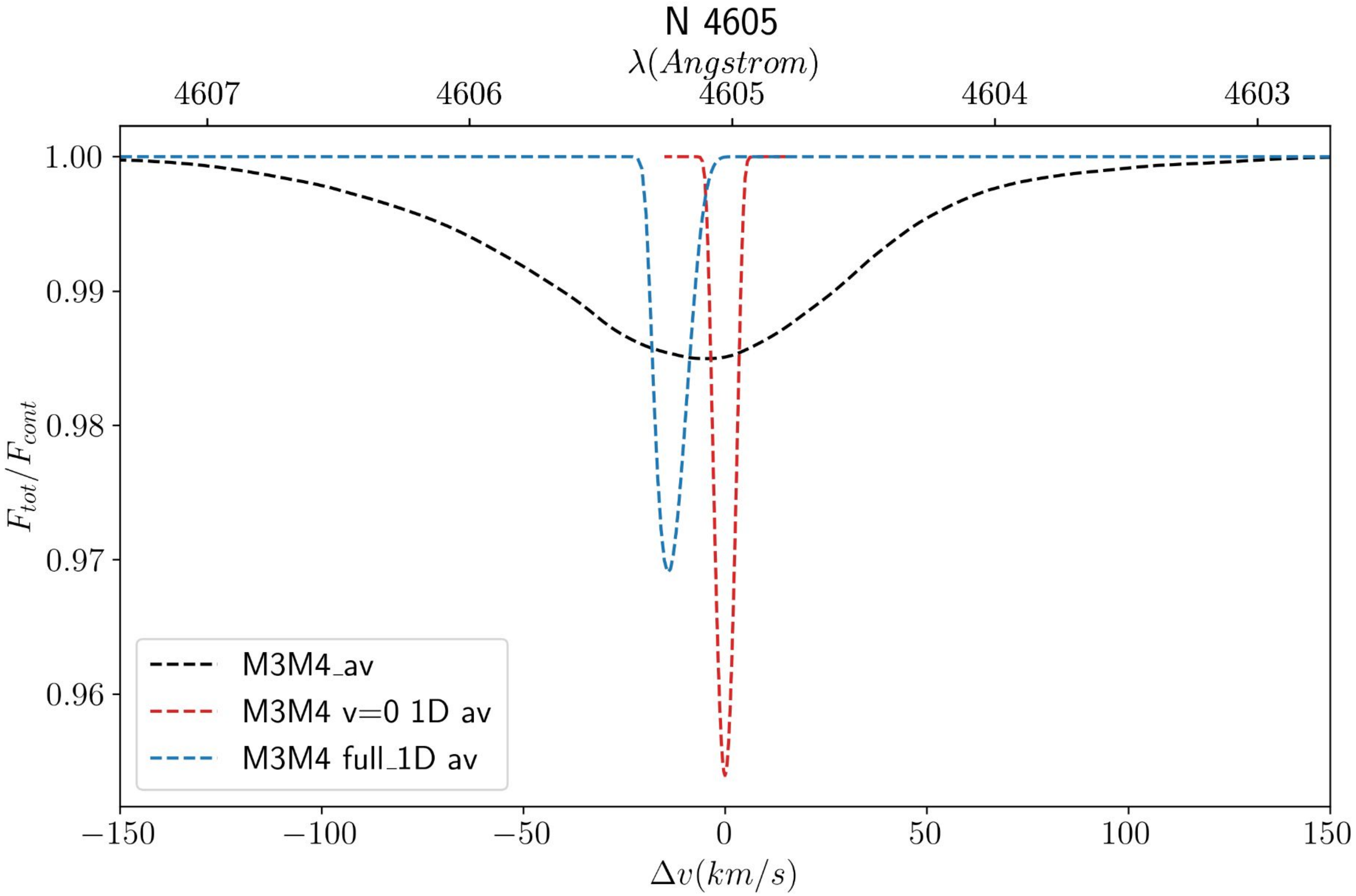

He 6529
$\lambda(Angstrom)$
6532
6530
6528
6526
1.00
0.95
0.90
0.85
0.80
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$

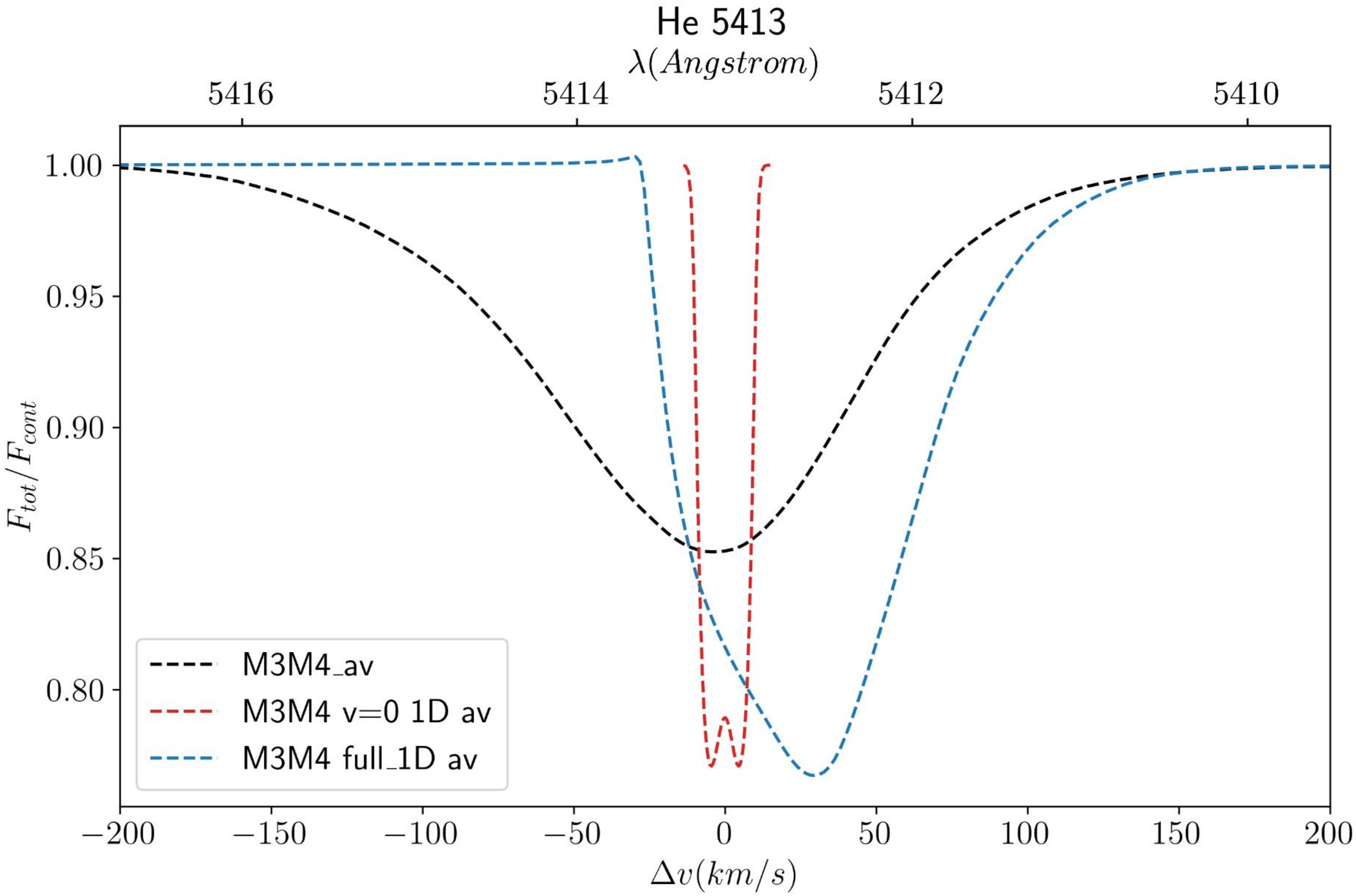

He 4201
$\lambda(Angstrom)$
4203
4202
4201
4200
4199
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
0.75
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av

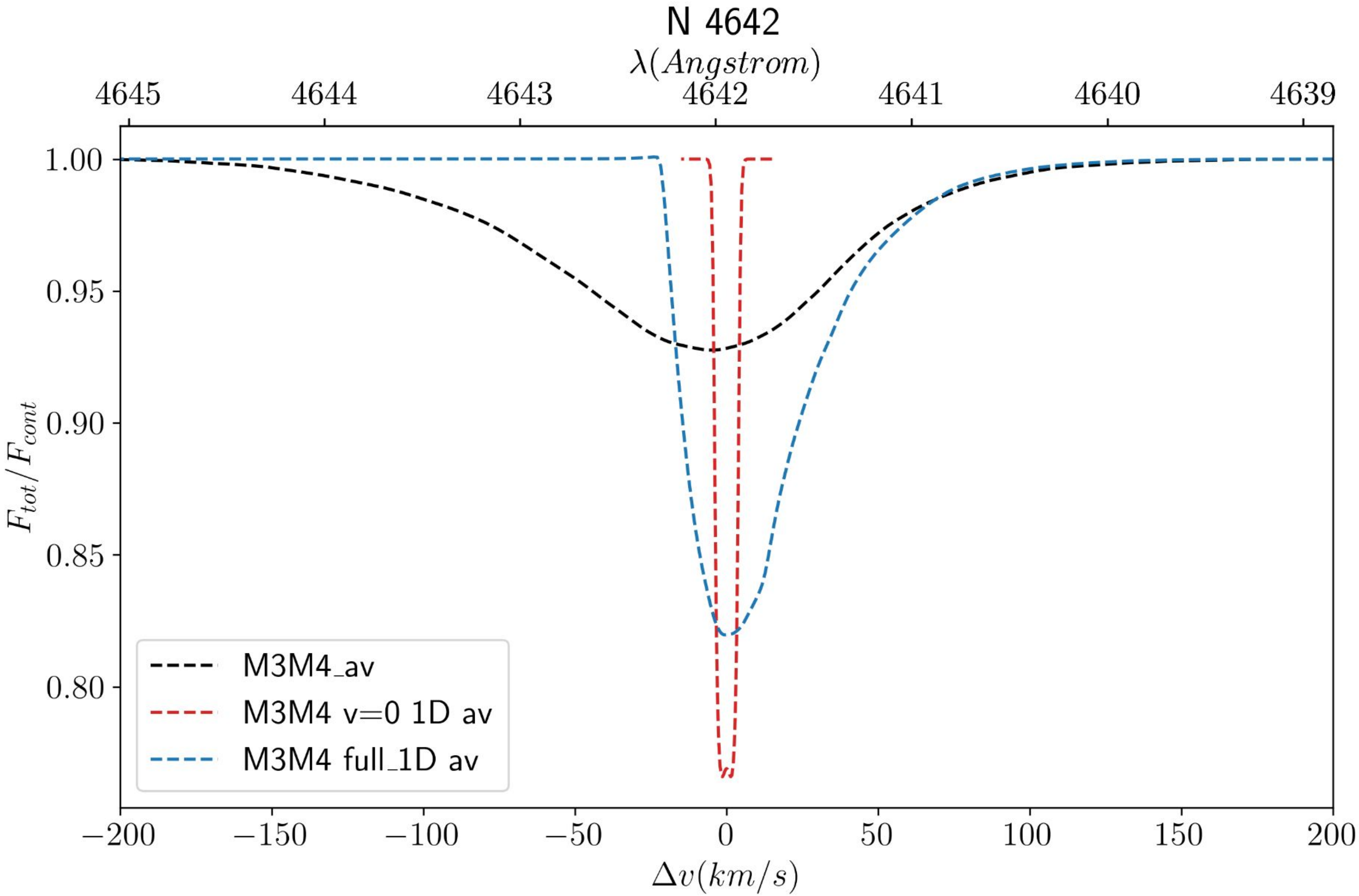

He 4473
$\lambda(Angstrom)$
4475
4474
4473
4472
4471
4470
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
0.75
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av

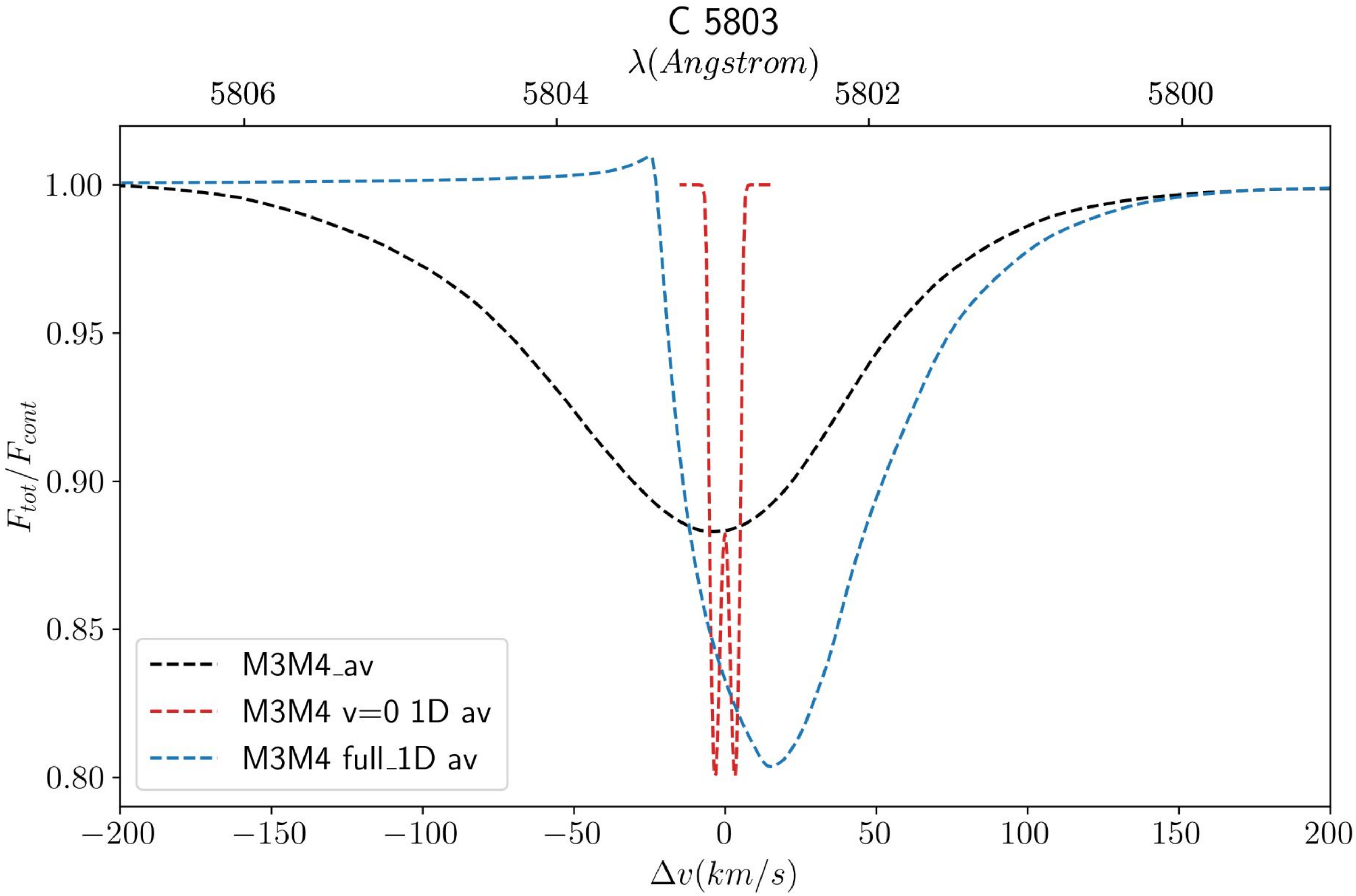

He 4687
$\lambda(Angstrom)$
4690
4688
4686
4684
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
0.75
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−300
−200
−100
0
100
200
300
$\Delta v(km/s)$

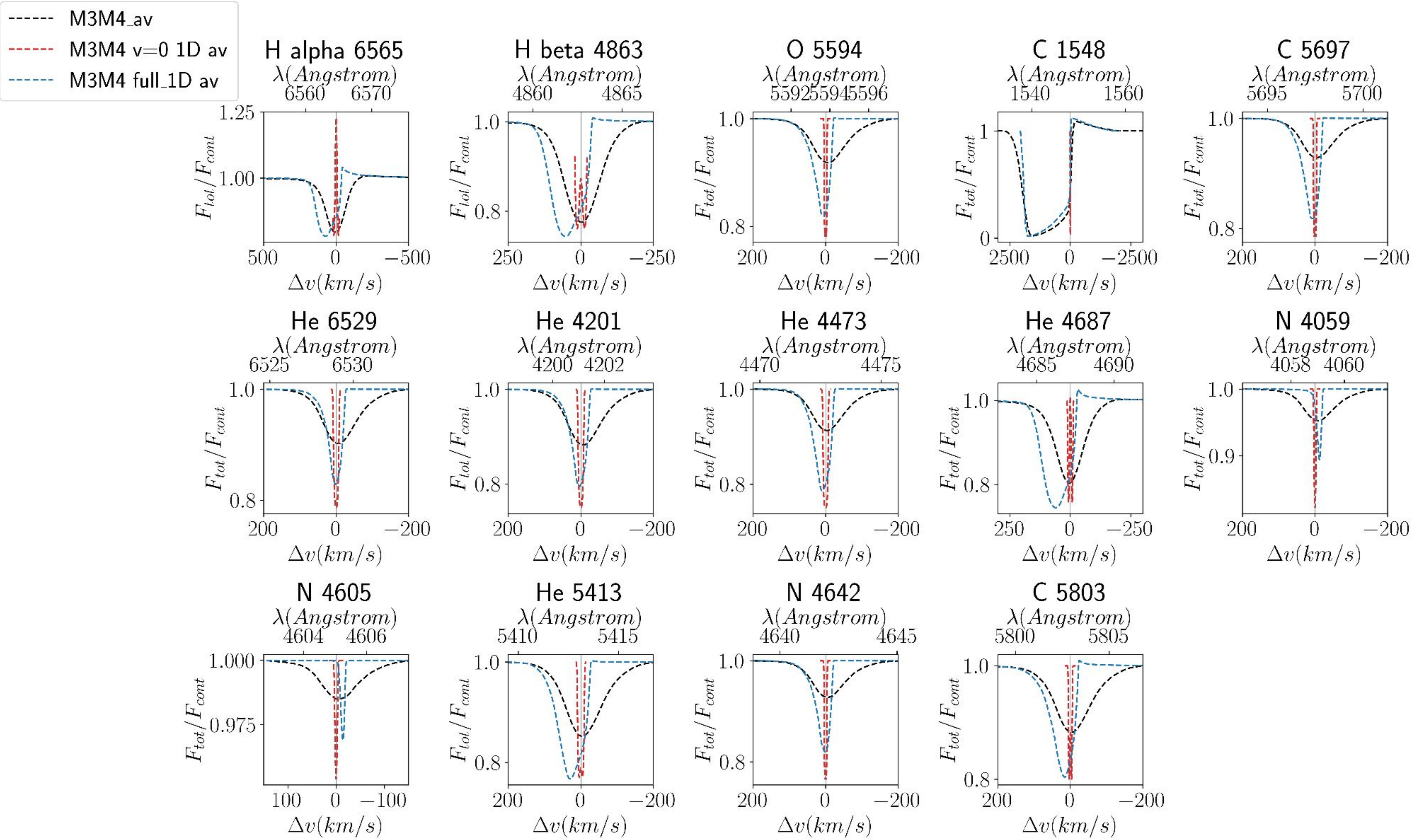

N 4059
λ(Angstrom)
4061
4060
4059
4058
4057
1.000
0.975
0.950
0.925
0.900
0.875
0.850
0.825
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−150
−100
−50
0
50
100
150
200
Δv(km/s)


N 4605
λ(Angstrom)
4607
4606
4605
4604
4603
1.00
0.99
0.98
0.97
0.96
F_tot/F_cont
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−150
−100
−50
0
50
100
150
Δv(km/s)


He 5413
$\lambda(Angstrom)$
5416
5414
5412
5410
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$

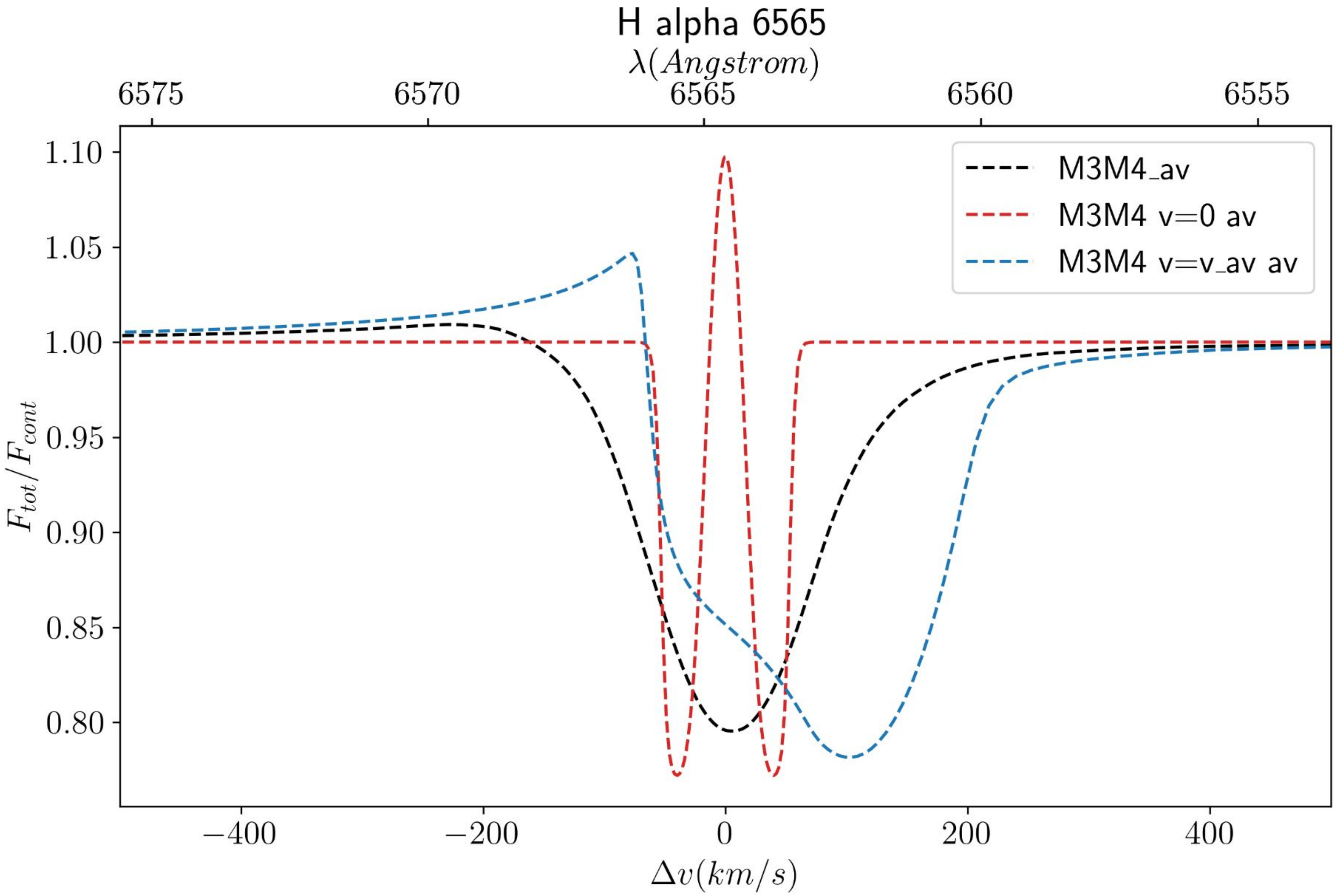

N 4642
$\lambda(Angstrom)$
4645
4644
4643
4642
4641
4640
4639
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$


C 5803
$\lambda(Angstrom)$
5806
5804
5802
5800
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av

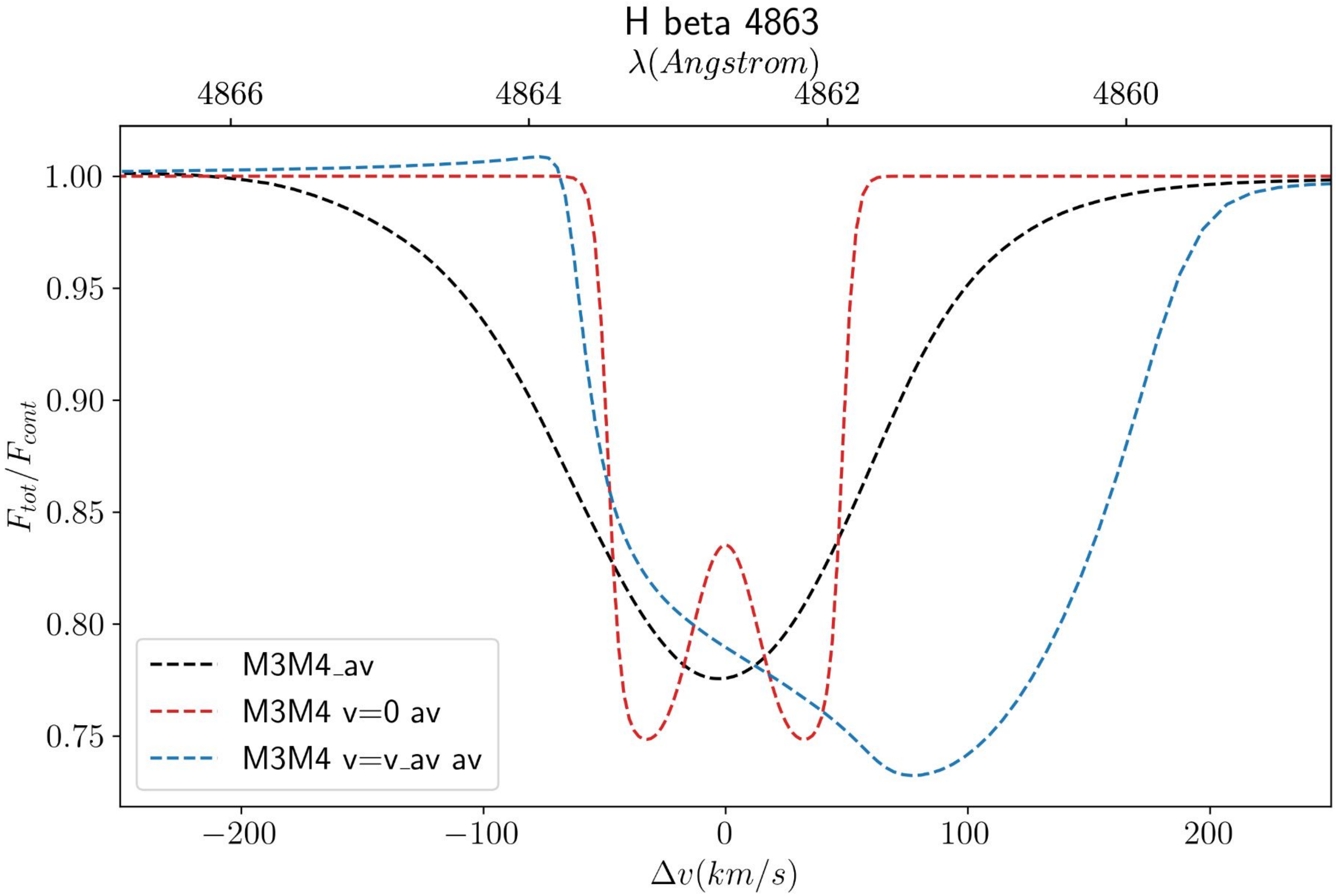

M3M4_av
M3M4 v=0 1D av
M3M4 full_1D av
H alpha 6565
H beta 4863
O 5594
C 1548
C 5697
He 6529
He 4201
He 4473
He 4687
N 4059
N 4605
He 5413
N 4642
C 5803
λ(Angstrom)
6560
6570
4860
4865
5592
5594
5596
1540
1560
5695
5700
6525
6530
4200
4202
4470
4475
4685
4690
4058
4060
4604
4606
5410
5415
4640
4645
5800
5805
F_{tot}/F_{cont}
1.25
1.00
1.0
0.9
0.8
1
0
1.000
0.975
500
0
−500
250
−250
200
−200
2500
−2500
100
−100
Δv(km/s)

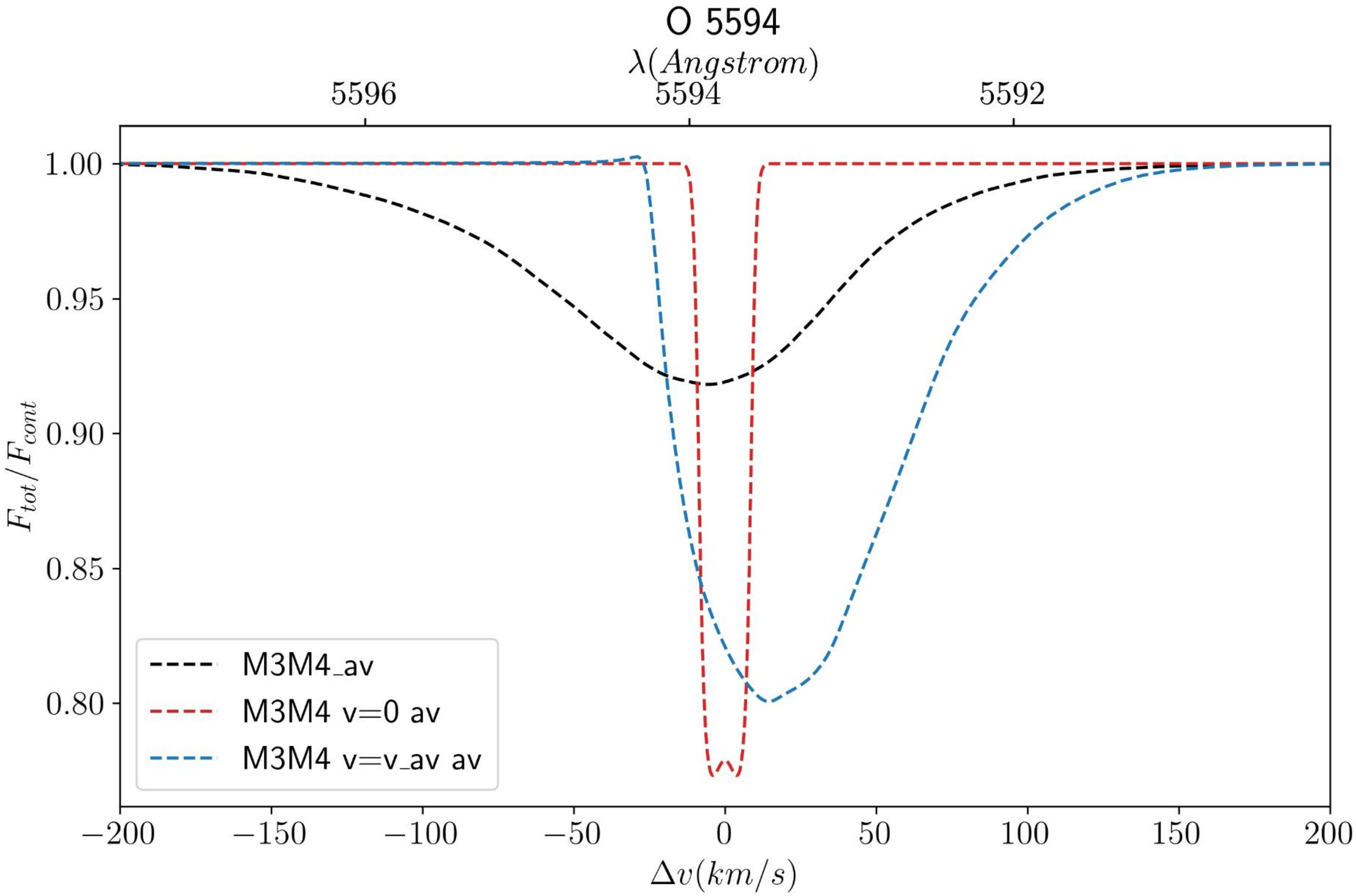
V = 0 averaged in spec

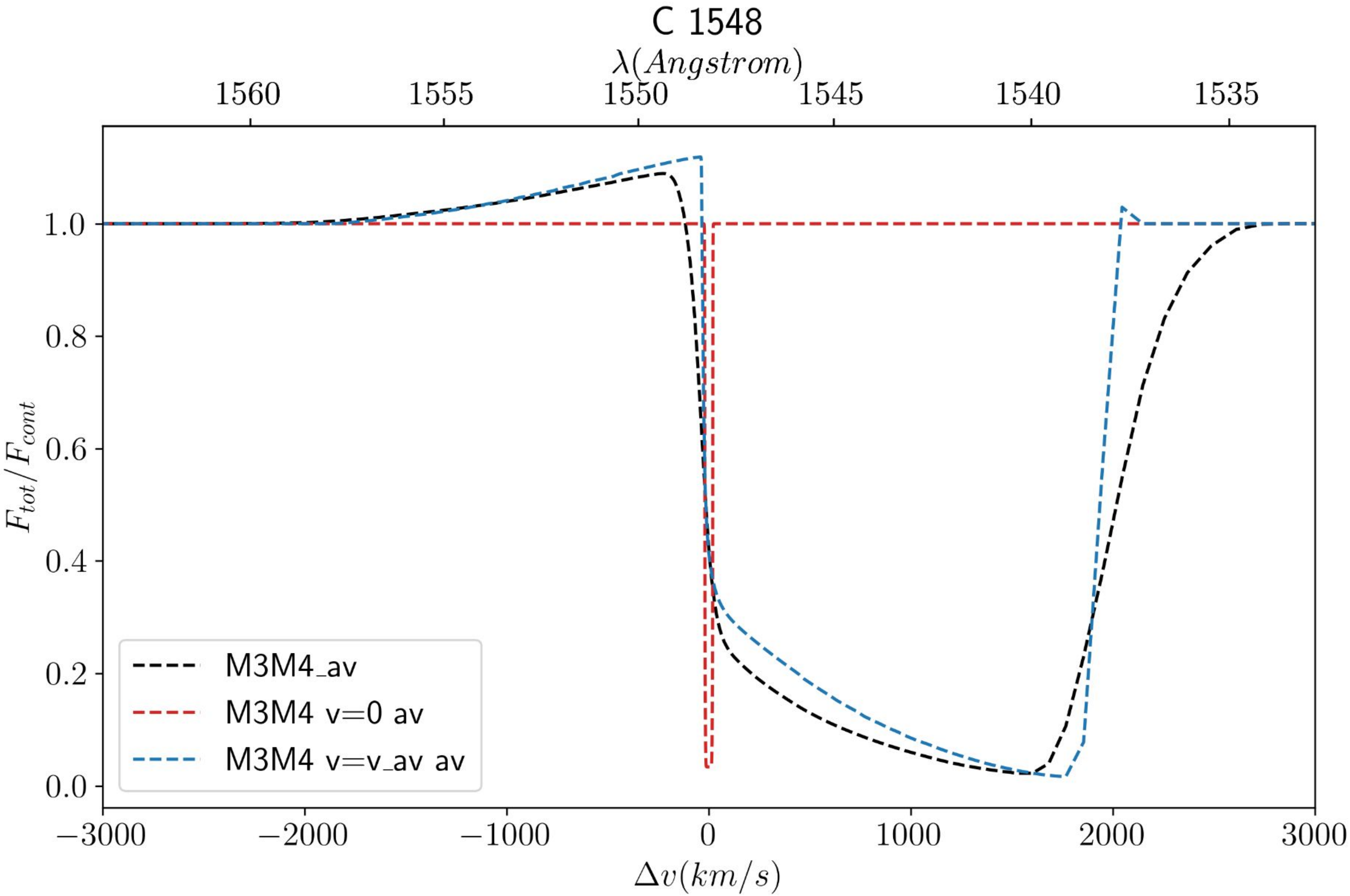
V = V_av averaged in spec

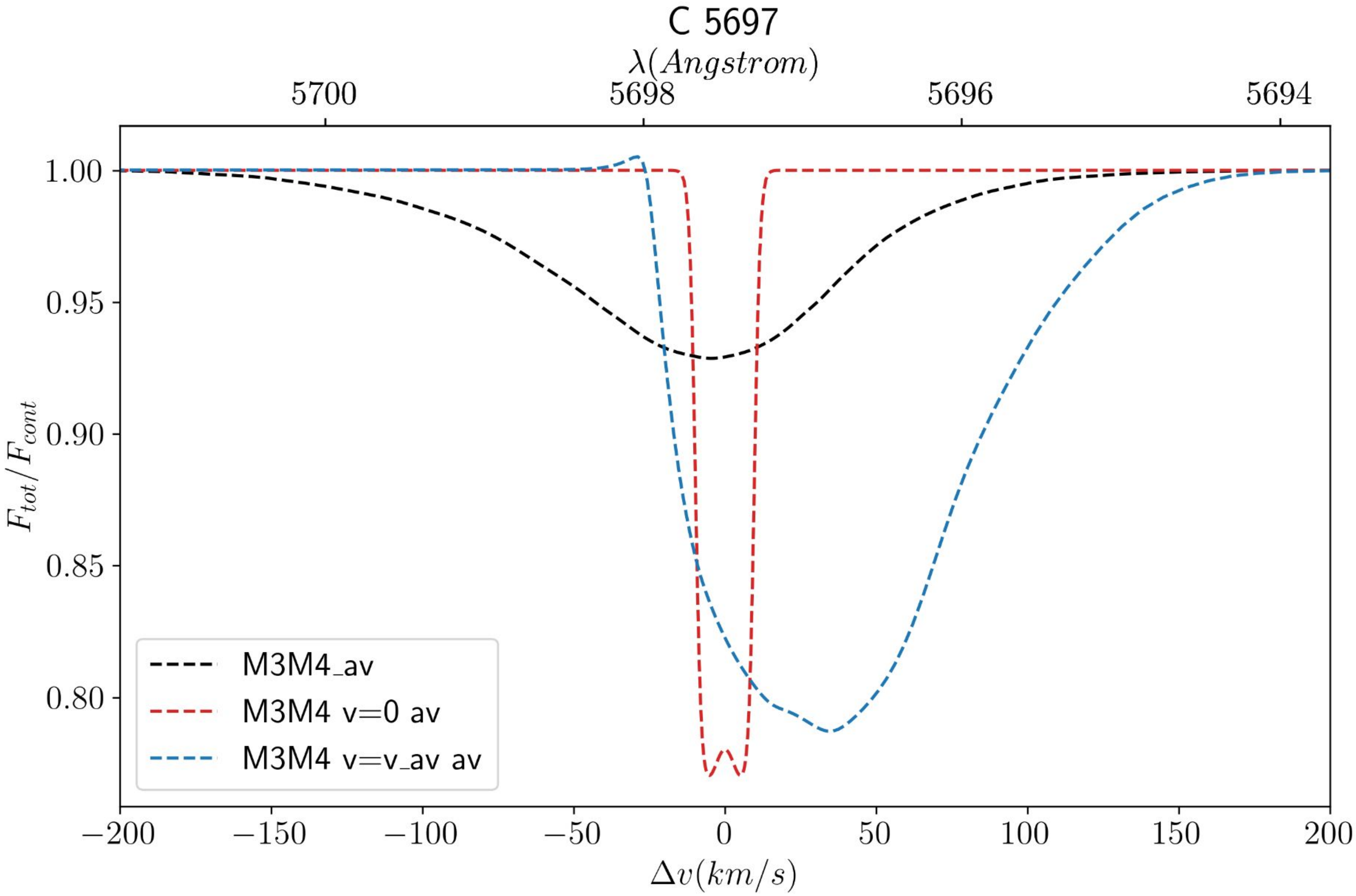


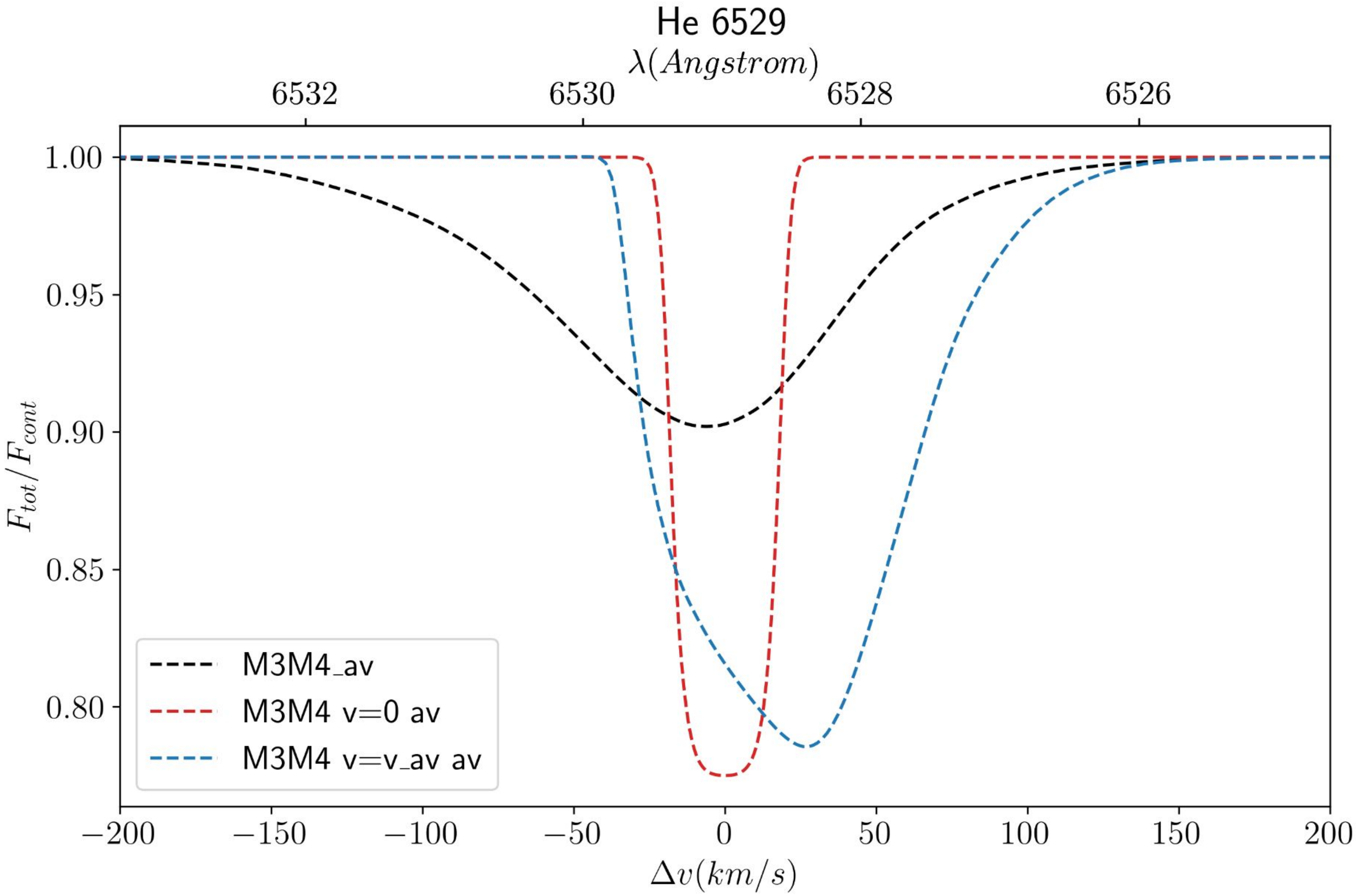
H alpha 6565
$\lambda(Angstrom)$
6575
6570
6565
6560
6555
F_{tot}/F_{cont}
1.10
1.05
1.00
0.95
0.90
0.85
0.80
−400
−200
0
200
400
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av

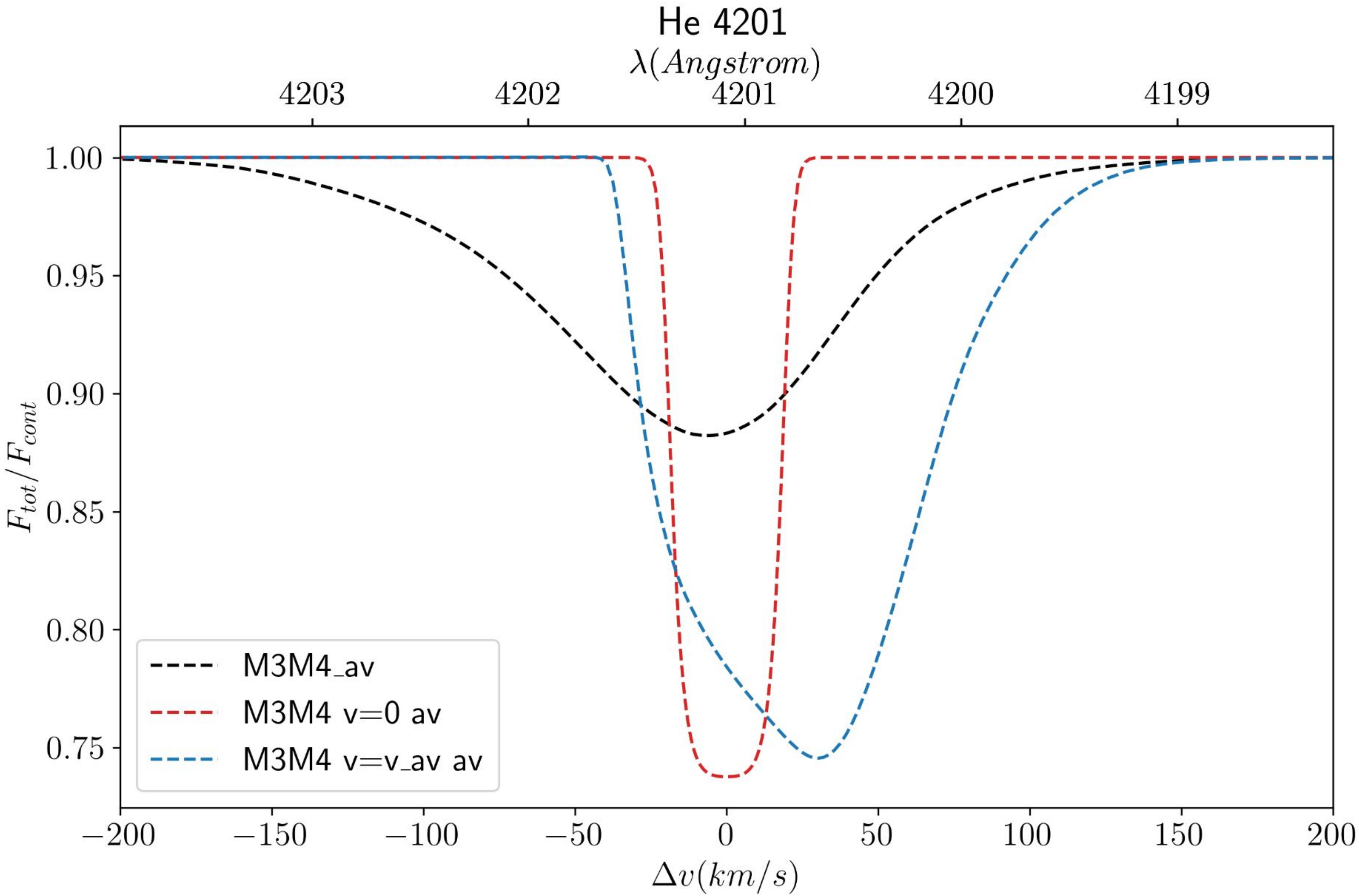

H beta 4863
$\lambda(Angstrom)$
4866
4864
4862
4860
1.00
0.95
0.90
0.85
0.80
0.75
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−100
0
100
200
$\Delta v(km/s)$

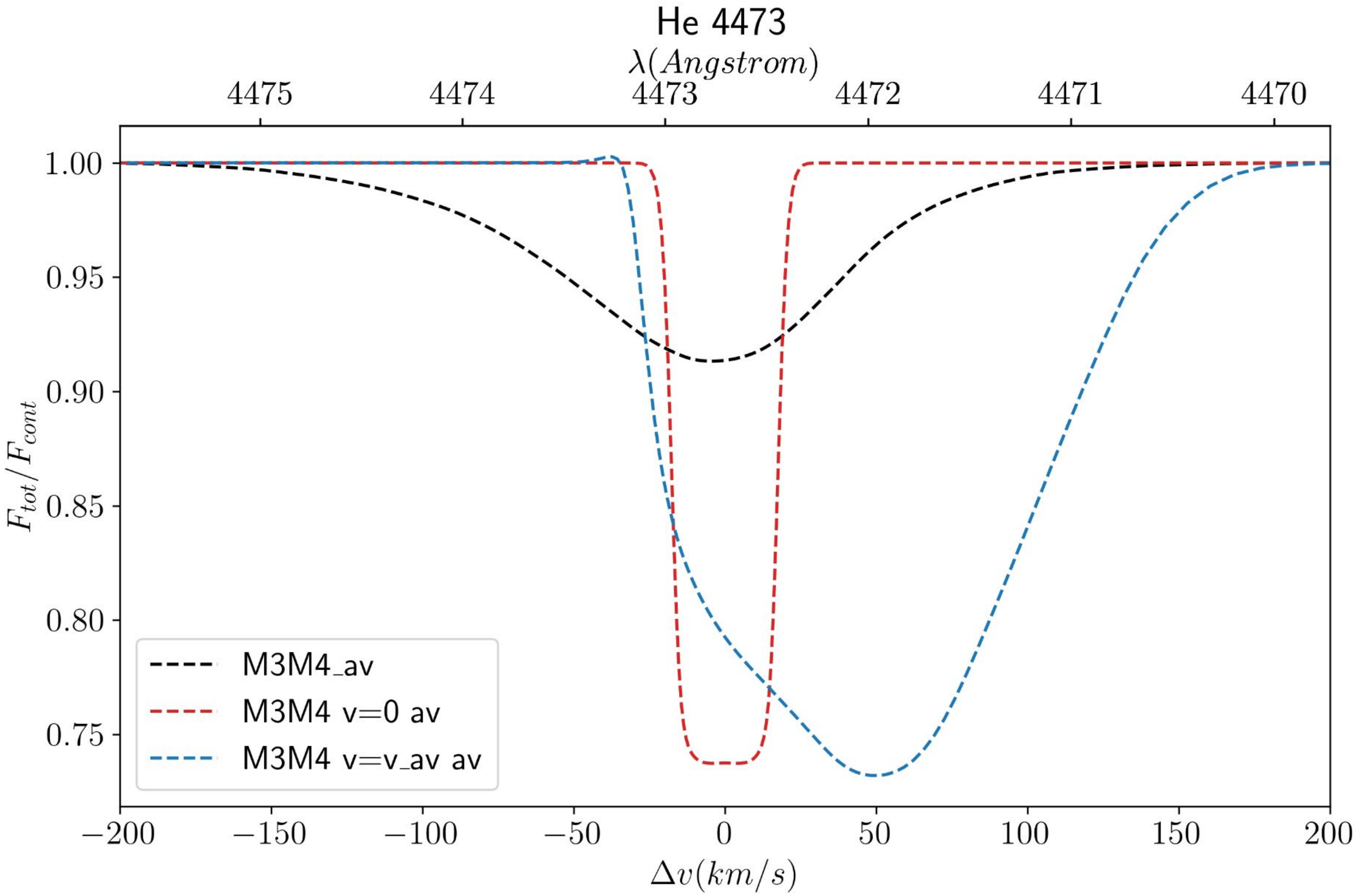

O 5594
$\lambda(Angstrom)$
5596
5594
5592
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av

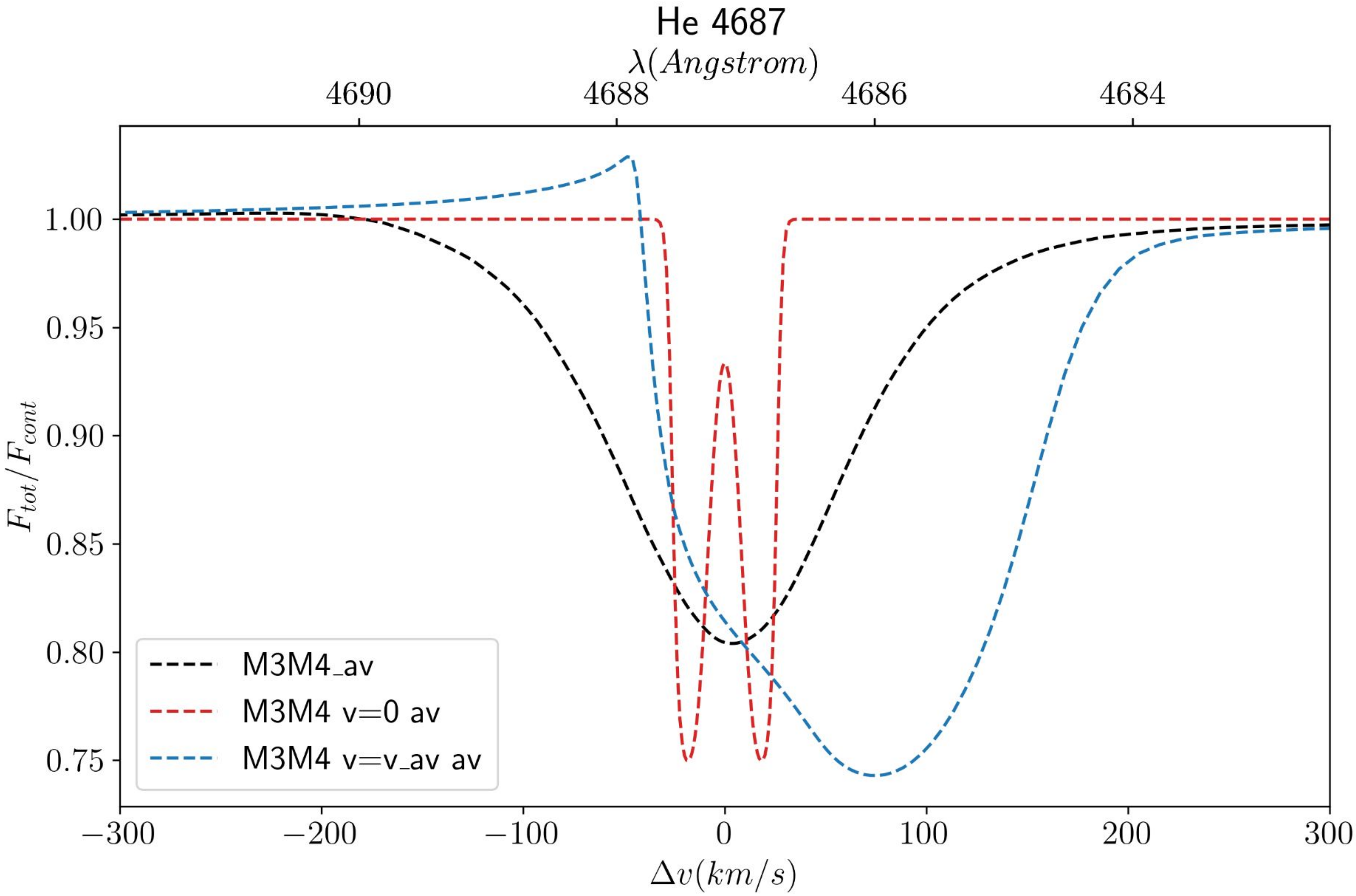

C 1548
$\lambda(Angstrom)$
1560
1555
1550
1545
1540
1535
F_{tot}/F_{cont}
0.0
0.2
0.4
0.6
0.8
1.0
−3000
−2000
−1000
0
1000
2000
3000
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av

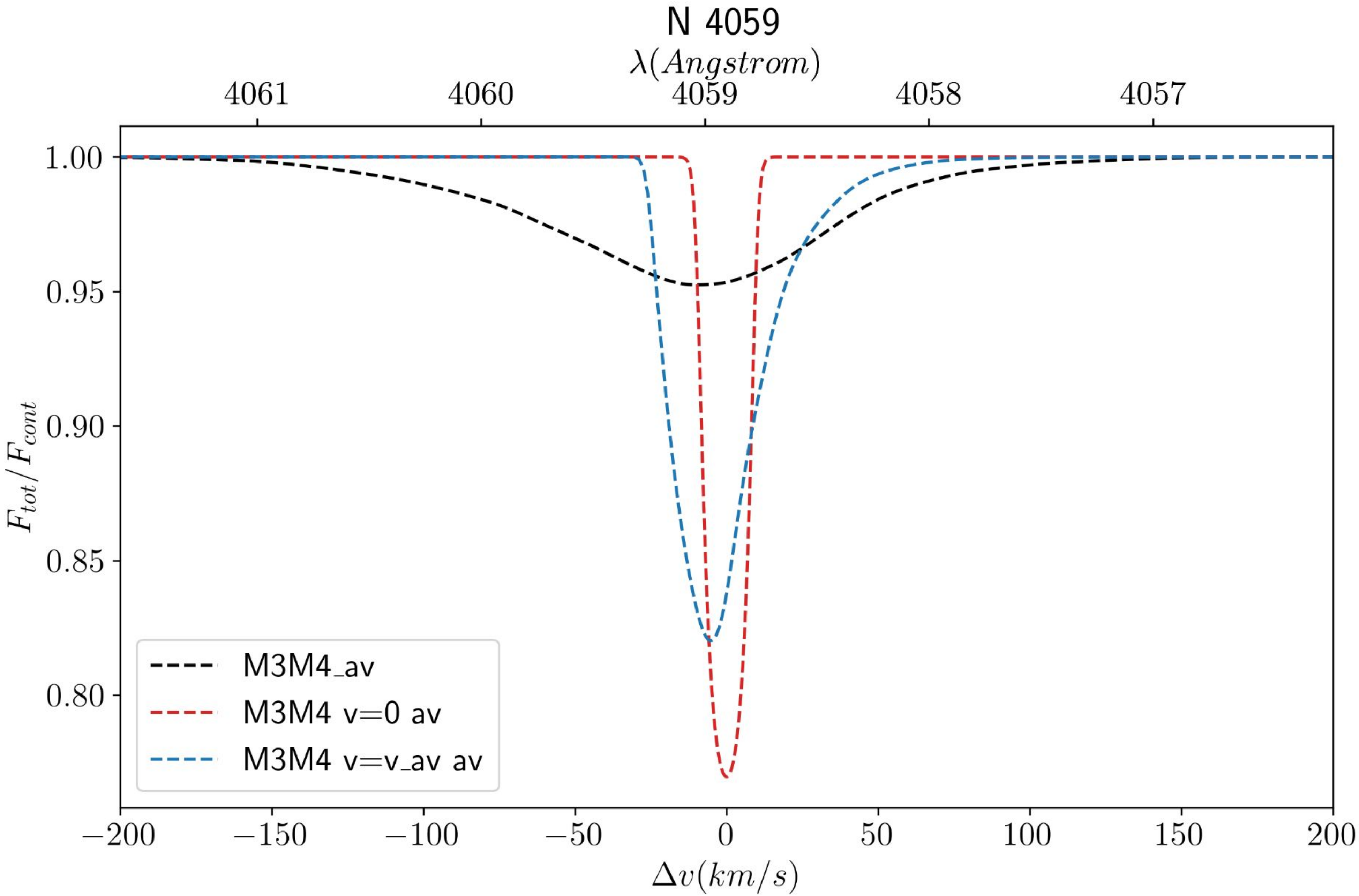

C 5697
$\lambda(Angstrom)$
5700
5698
5696
5694
1.00
0.95
0.90
0.85
0.80
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$

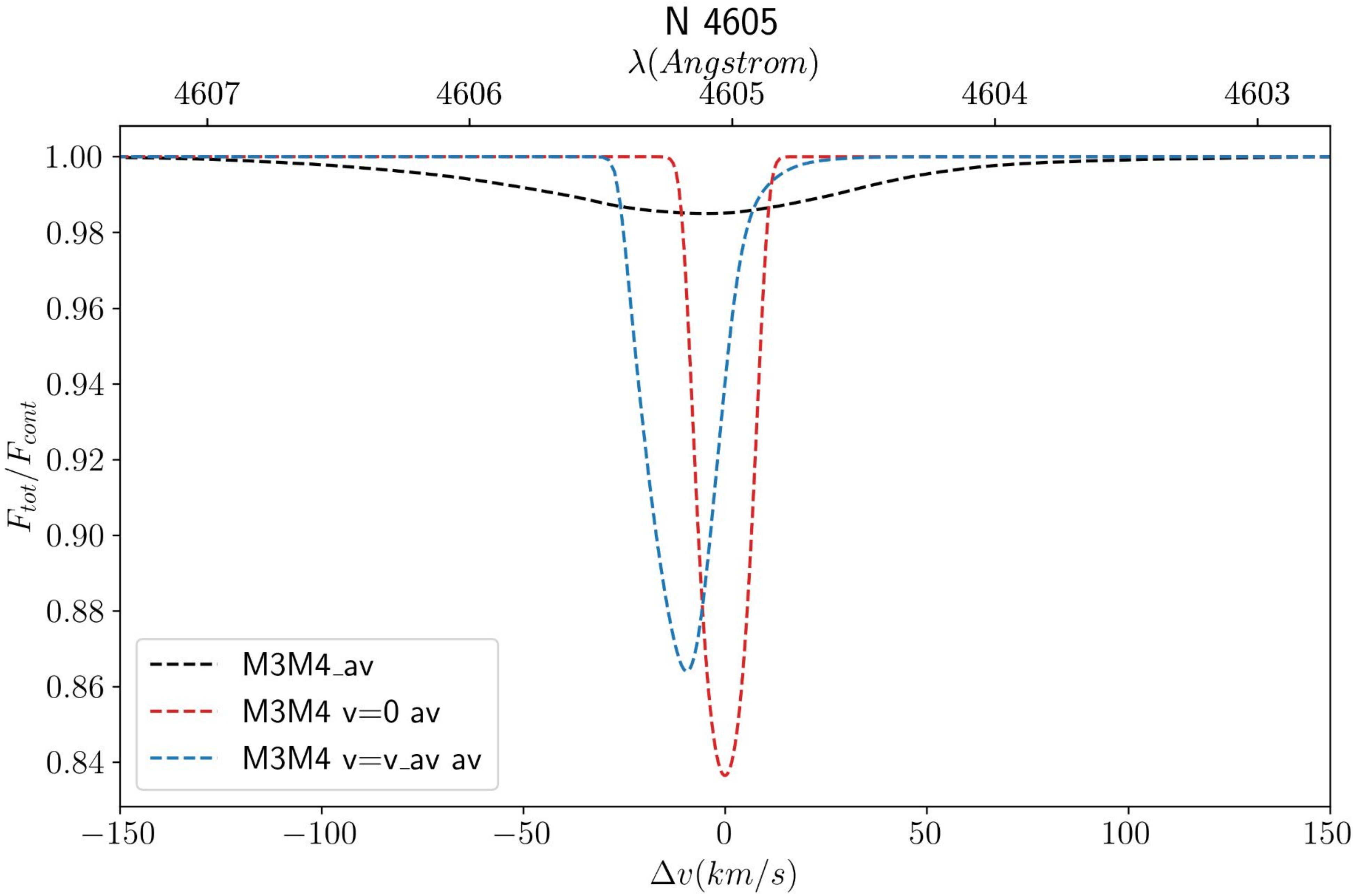

He 6529
λ(Angstrom)
6532
6530
6528
6526
1.00
0.95
0.90
0.85
0.80
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−150
−100
−50
0
50
100
150
200
Δv(km/s)

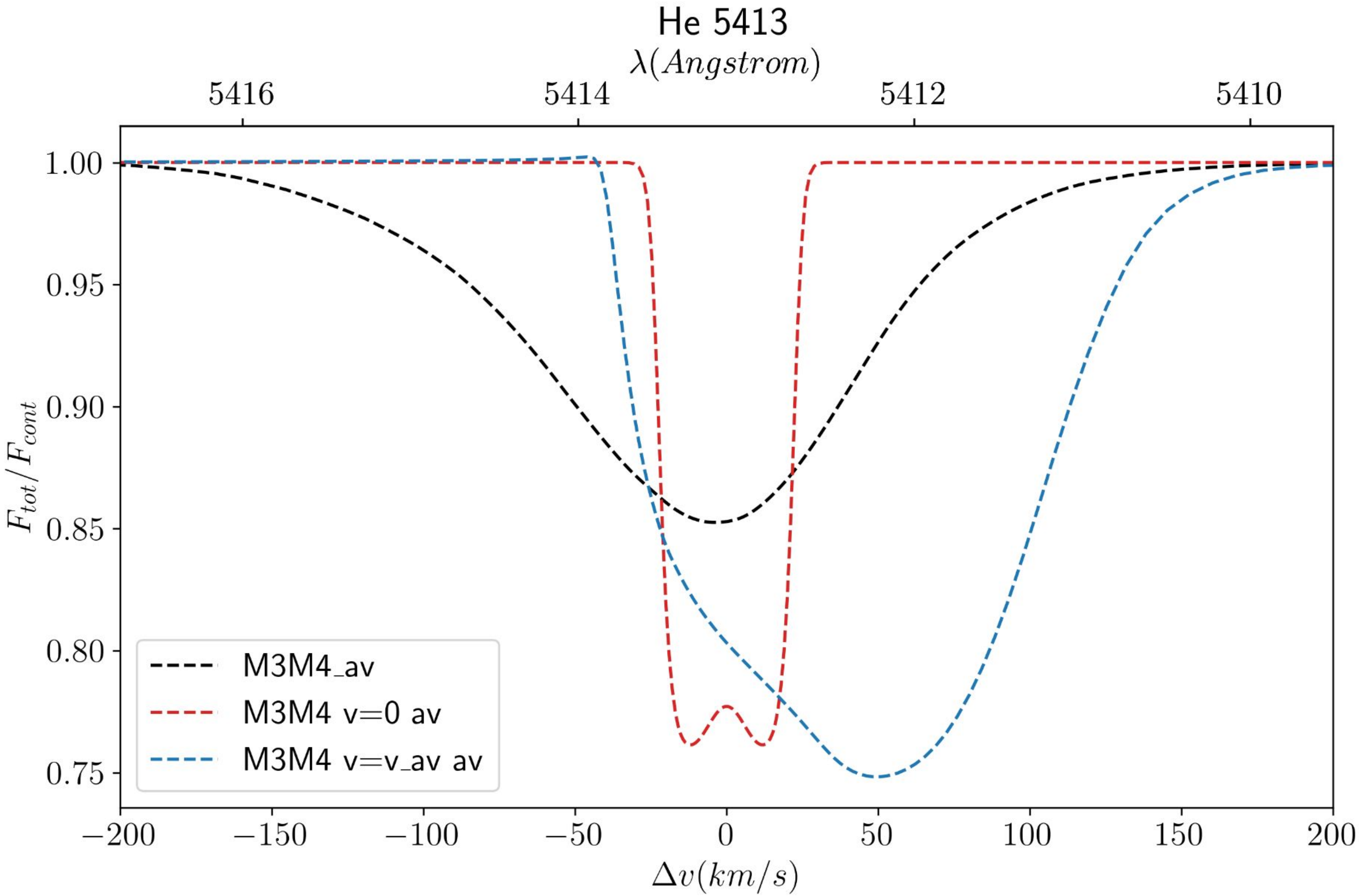

He 4201
$\lambda(Angstrom)$
4203
4202
4201
4200
4199
1.00
0.95
0.90
0.85
0.80
0.75
F_{tot}/F_{cont}
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av

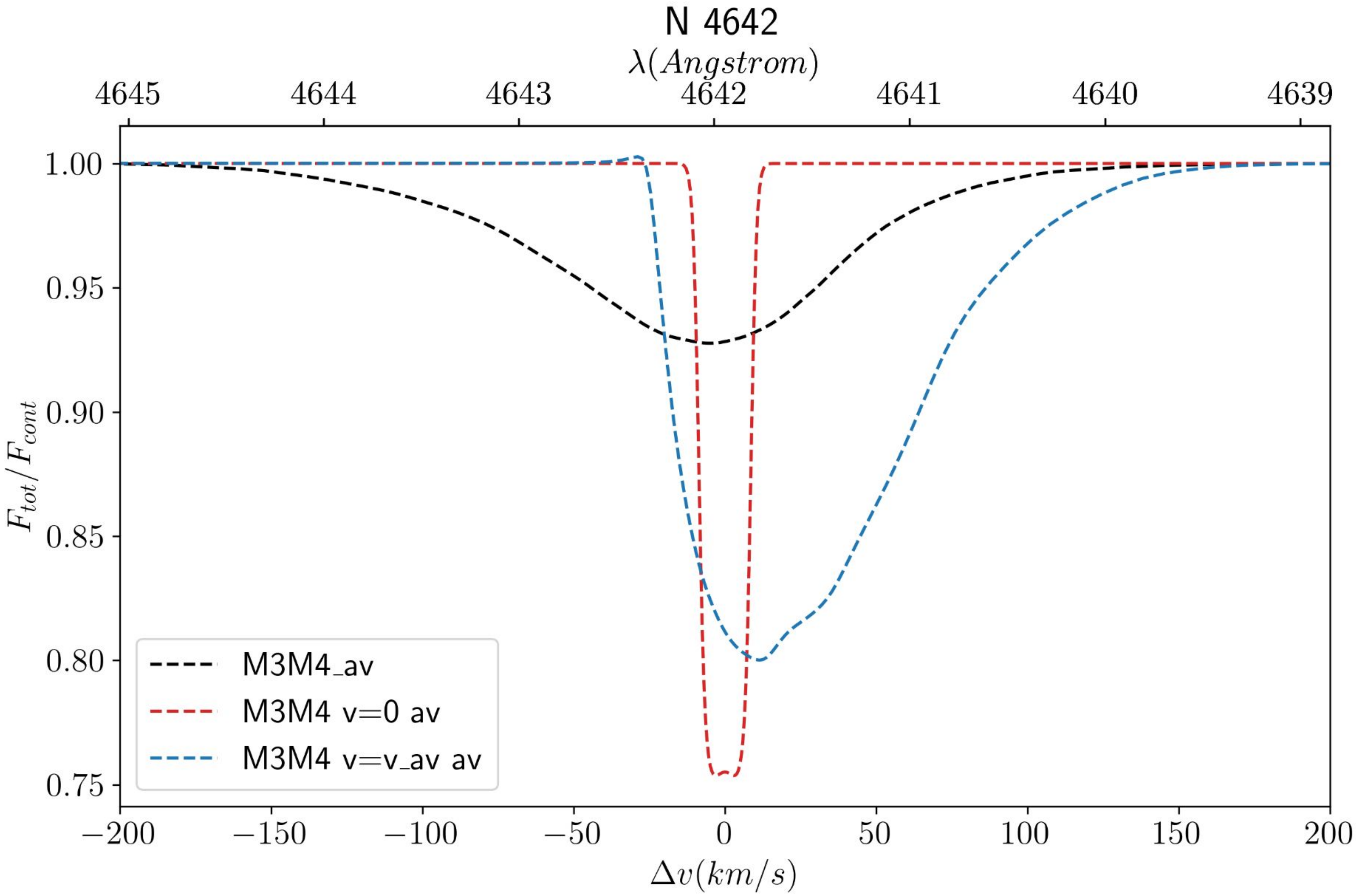

He 4473
$\lambda(Angstrom)$
4475
4474
4473
4472
4471
4470
1.00
0.95
0.90
0.85
0.80
0.75
F_{tot}/F_{cont}
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$

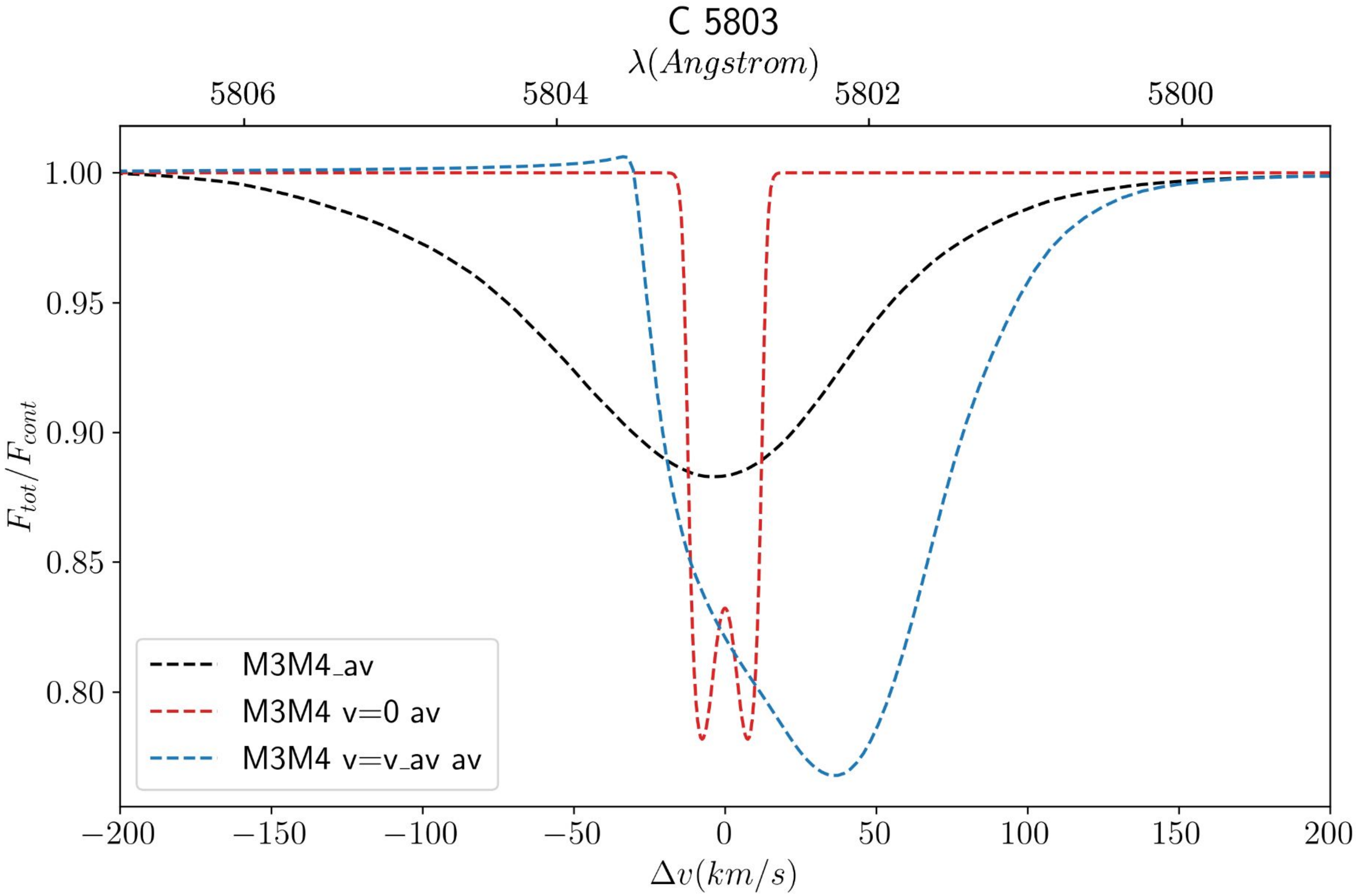

He 4687
λ(Angstrom)
4690
4688
4686
4684
F_tot/F_cont
1.00
0.95
0.90
0.85
0.80
0.75
−300
−200
−100
0
100
200
300
Δv(km/s)
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av

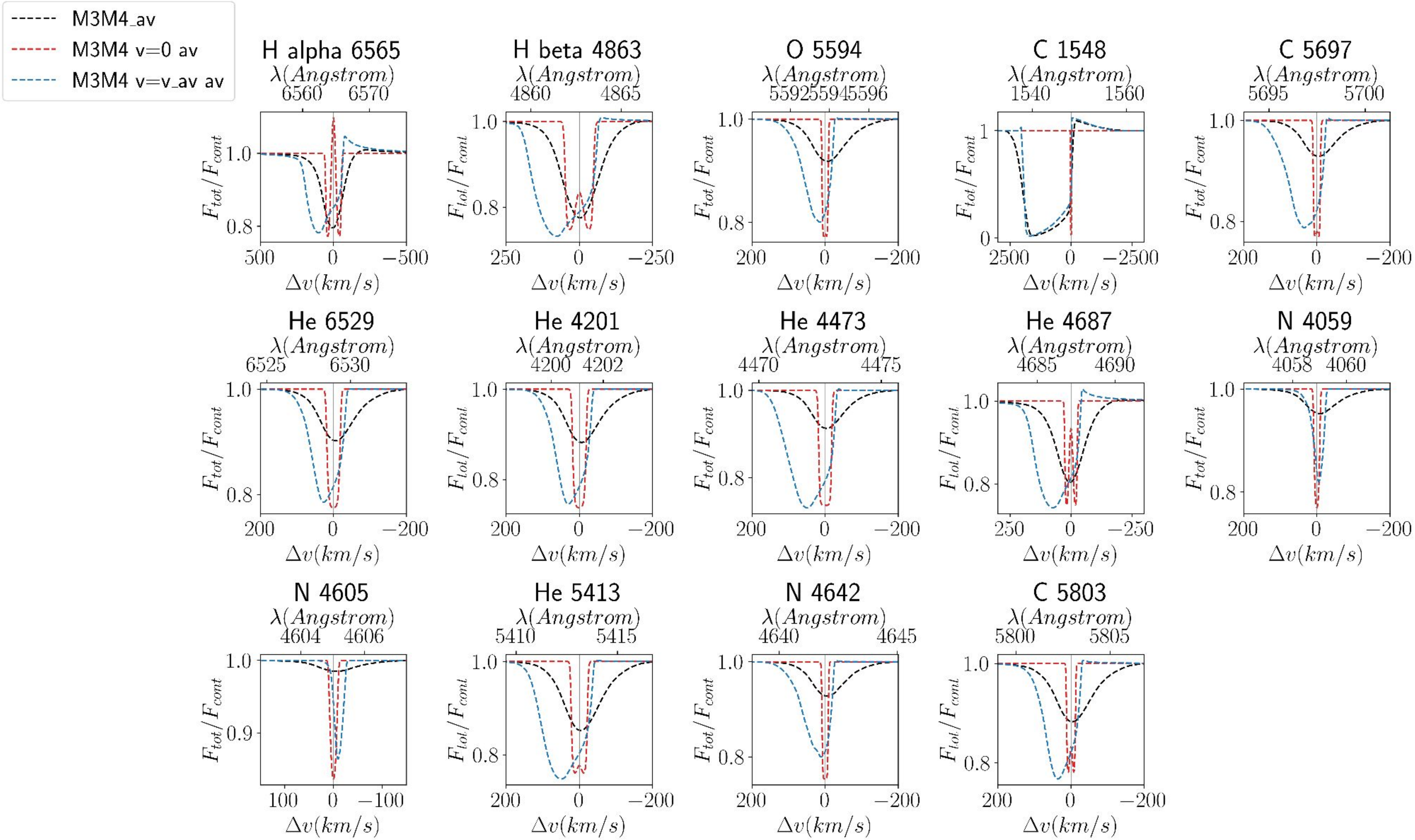

N 4059
$\lambda(Angstrom)$
4061
4060
4059
4058
4057
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$


N 4605
$\lambda(Angstrom)$
4607
4606
4605
4604
4603
F_{tot}/F_{cont}
1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−150
−100
−50
0
50
100
150
$\Delta v(km/s)$


He 5413
λ(Angstrom)
5416
5414
5412
5410
F_tot/F_cont
1.00
0.95
0.90
0.85
0.80
0.75
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
−200
−150
−100
−50
0
50
100
150
200
Δv(km/s)


N 4642
$\lambda(Angstrom)$
4645
4644
4643
4642
4641
4640
4639
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
0.75
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av


C 5803
$\lambda(Angstrom)$
5806
5804
5802
5800
F_{tot}/F_{cont}
1.00
0.95
0.90
0.85
0.80
−200
−150
−100
−50
0
50
100
150
200
$\Delta v(km/s)$
M3M4_av
M3M4 v=0 av
M3M4 v=v_av av


M3M4_av
M3M4 v=0 av
M3M4 v=v_av av
H alpha 6565
H beta 4863
O 5594
C 1548
C 5697
He 6529
He 4201
He 4473
He 4687
N 4059
N 4605
He 5413
N 4642
C 5803
λ(Angstrom)
6560
6570
4860
4865
5592
5594
5596
1540
1560
5695
5700
6525
6530
4200
4202
4470
4475
4685
4690
4058
4060
4604
4606
5410
5415
4640
4645
5800
5805
F_tot/F_cont
1.0
0.9
0.8
1
0
Δv(km/s)
500
0
−500
250
−250
200
−200
2500
−2500
100
−100

Which techniques and advantages

3D model: Moving away from 'free parameter heaven/hell'

Input parameters (1D and 3D):

M, L, R, [Fe/H], v sin i

Additional (free) parameters in 1D:

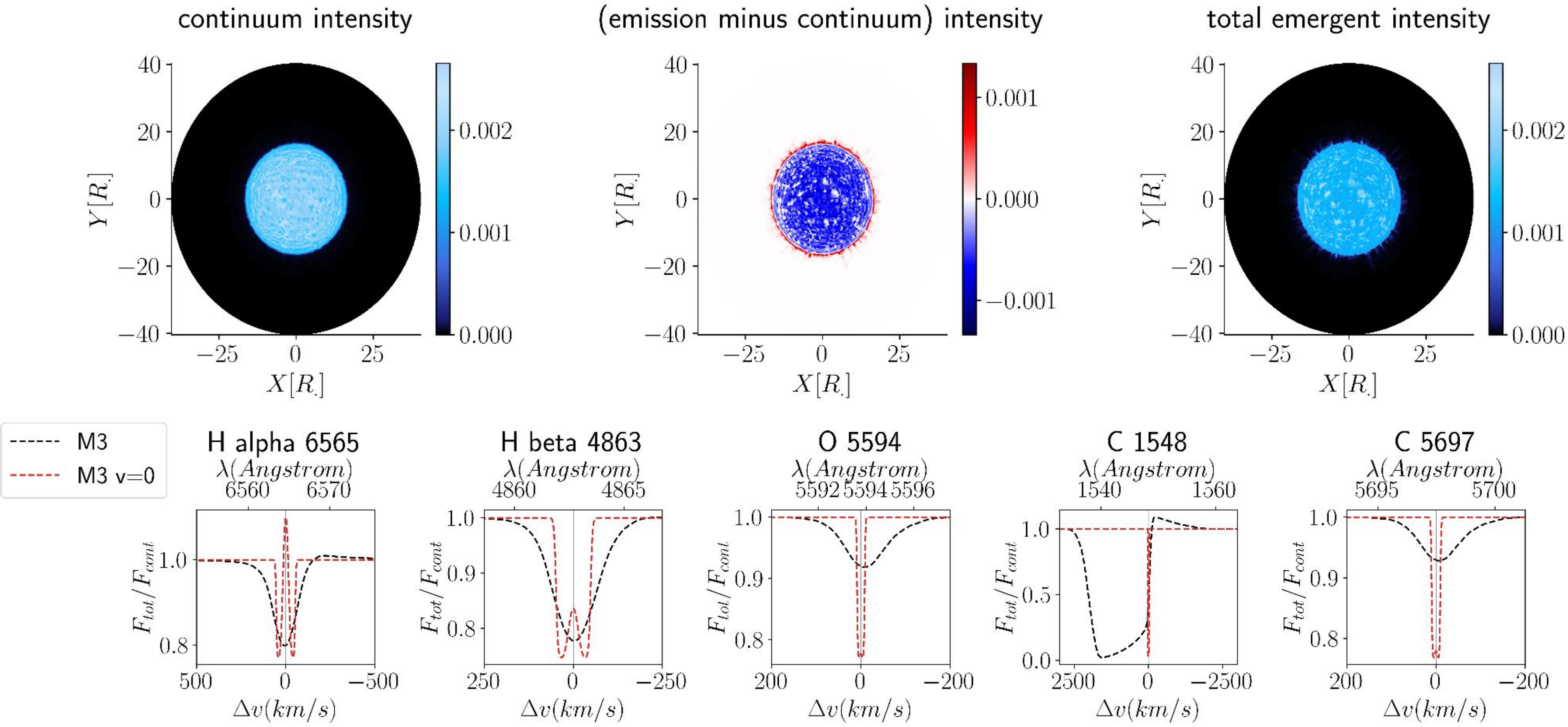
- Global wind parameters: $\dot{M}$, v∞, β
- Vmic, Vmac, wind structure (fcl, fvel, vcl, …)

Parameters defining the presented 3D models:

M, L, R, [Fe/H]

No micro-/macroturbulence added in spectral line formation!

Surface brightness/emergent flux profiles



Toward spectral analysis with 3D model atmospheres
Lara Delbroek

- 3D-RT package to explore effects on spectra (Multi-D O-star atmosphere with wind models)
- Very turbulent atmosphere, large velocity fields and density variations also in photosphere
- no micro- or macroturbulence needed
- Observed (high-resolution, high S/N) line widths, shapes, and shifts might be used as critical tests
- Relative 3D effects on chemical abundance and stellar parameter derivation to be explored
  (See also talk by Gemma Gonzalez)