rtdpy: A python package for residence time distributions

Matthew H. Flamm[1]

1 US Data Science and Applied Mathematics, Merck & Co., Inc., Kenilworth, NJ, USA

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Software

- Review
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Summary

Residence time distributions (RTDs) are used to understand nonideality in chemical reactors and other continuous flow through steps (Levenspiel, 1999). Applications include chemical reaction conversion (Danckwerts, 1953), pipeline mixing (Levenspiel, 1958), and material traceability (Engisch & Muzzio, 2016). RTDs also characterize flow patterns in stream flows (Haggerty, Wondzell, & Johnson, 2002) with applications in transport of pollutants (Kirchner, Feng, & Neal, 2000).

A residence time distribution, also known as the exit-age function, is the distribution of time material takes to exit a volume once it enters. While some RTD models are nearly trivial to implement, some require numerical solutions to advection-diffusion partial differential equations. In many analyses, there is a need to combine multiple RTD models together, particularly for processes with mutliple unit operations. Common RTD analyses are output prediction given an input signal, frequency-space signal damping, and disturbance mapping.

`rtdpy` is a Python package that enables quick and easy computation and usage of RTD models. Current model functionality is focused on continuous process unit operations. RTD models include:

- N continually stirred tank reactors (NCSTR), AKA tanks-in-series
- Tube flow with axial dispersion
  - Large Peclet number assumption
  - Open-open boundary conditions
  - Closed-closed boundary conditions
- Plug flow reactor (PFR)
- Pure convection model
- Zusatz model
- Any arbitrary combinations of the above

Built-in functionalities for all RTD models include:

- The RTD itself
- Mean residence time
- Variance
- Frequency response
- Disturbance funnelplot
- Input signal convolution
- Step response

An example of using `rtdpy` is to generate a family of NCSTR models as shown in Figure 1.

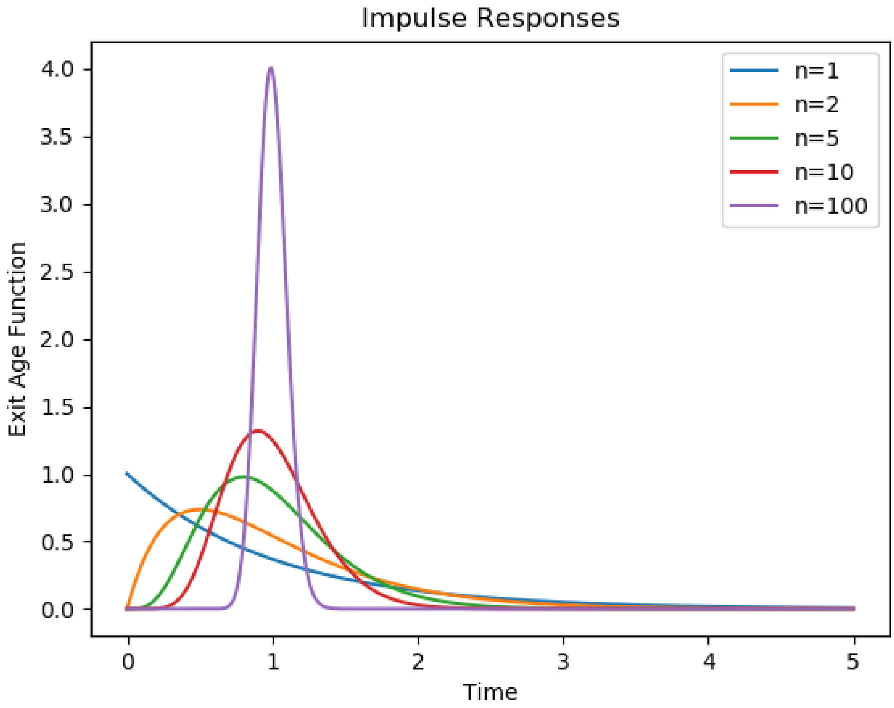

Figure 1: Family of NCSTR models.

```
import matplotlib.pyplot as plt
import rtdpy
for n in [1, 2, 5, 10, 100]:
    a = rtdpy.Ncstr(tau=1, n=n, dt=.001, time_end=5)
    plt.plot(a.time, a.exitage, label="n={}".format(n))
plt.legend()
plt.xlabel('Time')
plt.ylabel('Exit Age Function')
plt.title('Impulse Responses')
```

`rtdpy` is enabled by `numpy` and `scipy` packages. Documentation on all major functionality and all RTD models is included in the repository. Several examples of common workflows are also provided. The base RTD class is available for adding additional functionality. The RTD class can also be extended for future or user-defined RTD models.

References

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