

$$\frac{ds}{dt} = k_2 * es - k_1 * s * e$$

$$\frac{de}{dt} = (k_2 + k_3) * es - k_1 * s * e$$

$$\frac{des}{dt} = k_1 * s * e - (k_2 + k_3) * es$$

$$\frac{dp}{dt} = k_3 * es$$

python:

```

1. import numpy as np
2. import matplotlib.pyplot as plt
3.
4. def funcSt(s,e,es,p,k1,k2,k3):
5.     return k2 * es - k1 * s * e
6. def funcEt(s,e,es,p,k1,k2,k3):
7.     return (k2 + k3) * es - k1 * s * e
8. def funcEST(s,e,es,p,k1,k2,k3):
9.     return k1 * s * e - (k2 + k3) * es
10. def funcPt(s,e,es,p,k1,k2,k3):
11.     return k3 * es
12.
13. # RK4
14. t_ini = 0          # tmin
15. t_end = 0.5        # tmax
16. t_h = 1e-5         # 步进长度

```

17.

18. `t = np.linspace(t_ini, t_end, int((t_end-t_ini)/t_h+1))`

19. `s = t.copy()`

20. `e = t.copy()`

21. `es = t.copy()`

22. `p = t.copy()`

23.

24. `pt = t.copy()`

25.

26. `s[0] = 10.0`

27. `e[0] = 1.0`

28. `es[0] = 0`

29. `p[0] = 0`

30.

31. `k1 = 100`

32. `k2 = 600`

33. `k3 = 150`

34.

35. `for i in range(t.shape[0]-1):`

36. `h_i = t[i+1] - t[i]`

37.

38. `k1_s = funcSt(s[i],e[i],es[i],p[i],k1,k2,k3)`

39. $k1_e = \text{funcEt}(s[i], e[i], es[i], p[i], k1, k2, k3)$

40. $k1_es = \text{funcEST}(s[i], e[i], es[i], p[i], k1, k2, k3)$

41. $k1_p = \text{funcPt}(s[i], e[i], es[i], p[i], k1, k2, k3)$

42.

43. $k2_s = \text{funcSt}(s[i] + h_i/2.0 * k1_s, e[i], es[i], p[i], k1, k2, k3)$

44. $k2_e = \text{funcEt}(s[i], e[i] + h_i/2.0 * k1_e, es[i], p[i], k1, k2, k3)$

45. $k2_es = \text{funcEST}(s[i], e[i], es[i] + h_i/2.0 * k1_es, p[i], k1, k2, k3)$

46. $k2_p = \text{funcPt}(s[i], e[i], es[i], p[i] + h_i/2.0 * k1_p, k1, k2, k3)$

47.

48. $k3_s = \text{funcSt}(s[i] + h_i/2.0 * k2_s, e[i], es[i], p[i], k1, k2, k3)$

49. $k3_e = \text{funcEt}(s[i], e[i] + h_i/2.0 * k2_e, es[i], p[i], k1, k2, k3)$

50. $k3_es = \text{funcEST}(s[i], e[i], es[i] + h_i/2.0 * k2_es, p[i], k1, k2, k3)$

51. $k3_p = \text{funcPt}(s[i], e[i], es[i], p[i] + h_i/2.0 * k2_p, k1, k2, k3)$

52.

53.

54. $k4_s = \text{funcSt}(s[i] + h_i/2.0 * k3_s, e[i], es[i], p[i], k1, k2, k3)$

55. $k4_e = \text{funcEt}(s[i], e[i] + h_i/2.0 * k3_e, es[i], p[i], k1, k2, k3)$

56. $k4_es = \text{funcEST}(s[i], e[i], es[i] + h_i/2.0 * k3_es, p[i], k1, k2, k3)$

57. $k4_p = \text{funcPt}(s[i], e[i], es[i], p[i] + h_i/2.0 * k3_p, k1, k2, k3)$

58.

59. $s[i+1] = s[i] + h_i/6.0 * (k1_s + 2.0 * k2_s + 2.0 * k3_s + k4_s)$

60. $e[i+1] = e[i] + h_i/6.0 * (k1_e + 2.0 * k2_e + 2.0 * k3_e + k4_e)$

```
61. es[i+1] = es[i] + h_i/6.0*(k1_es + 2.0 * k2_es + 2.0* k3_es + k4_es)
```

```
62. p[i+1] = p[i] + h_i/6.0*(k1_p + 2.0 * k2_p + 2.0* k3_p + k4_p)
```

```
63.
```

```
64. pt[i] = k1_p
```

```
65.
```

```
66.pt =np.abs(pt)
```

```
67. ### 画图
```

```
68.plt.subplot(1, 4, 1)
```

```
69.plt.plot(t, s, 'b', label='RK4')
```

```
70.plt.legend()
```

```
71.plt.xlabel('t')
```

```
72.plt.ylabel('s')
```

```
73.plt.title('s-t')
```

```
74.
```

```
75.plt.subplot(1, 4, 2)
```

```
76.plt.plot(t, e, 'b', label='RK4')
```

```
77.plt.legend()
```

```
78.plt.xlabel('t')
```

```
79.plt.ylabel('e')
```

```
80.plt.title('e-t')
```

```
81.
```

```
82.plt.subplot(1, 4, 3)
```

```
83. plt.plot(t, es, 'b', label='RK4')
```

```
84. plt.legend()
```

```
85. plt.xlabel('t')
```

```
86. plt.ylabel('es')
```

```
87. plt.title('es-t')
```

```
88.
```

```
89. plt.subplot(1, 4, 4)
```

```
90. plt.plot(t, p, 'b', label='RK4')
```

```
91. plt.legend()
```

```
92. plt.xlabel('t')
```

```
93. plt.ylabel('p')
```

```
94. plt.title('p-t')
```

```
95. plt.show()
```

```
96.
```

```
97. plt.plot(s, pt, 'b', label='RK4')
```

```
98. plt.legend()
```

```
99. plt.xlabel('s')
```

```
100. plt.ylabel('v')
```

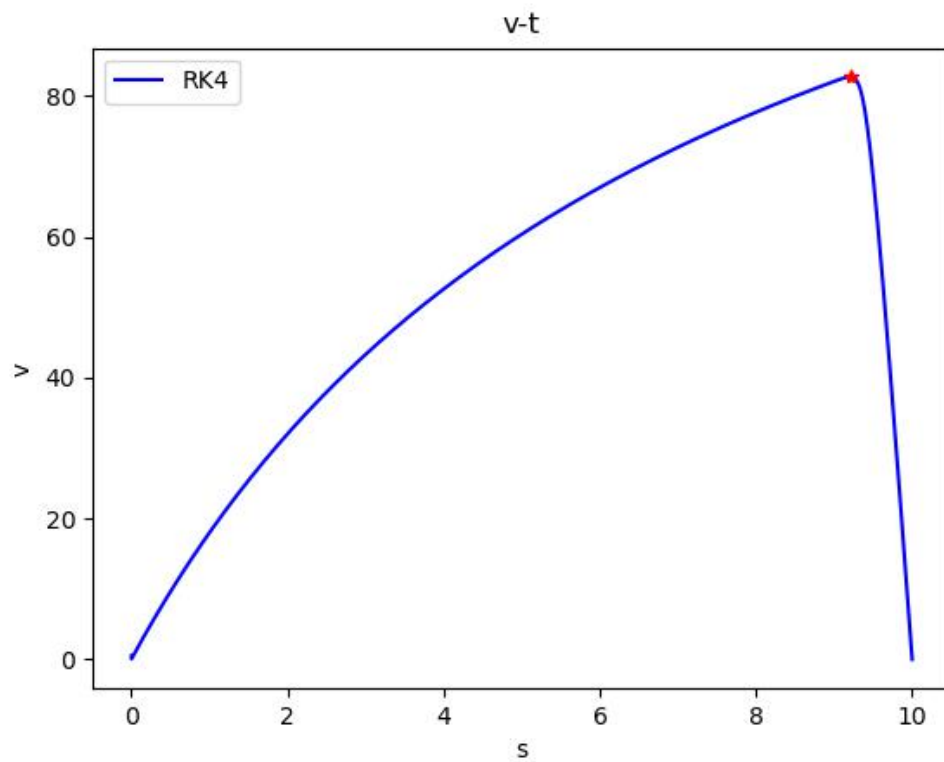
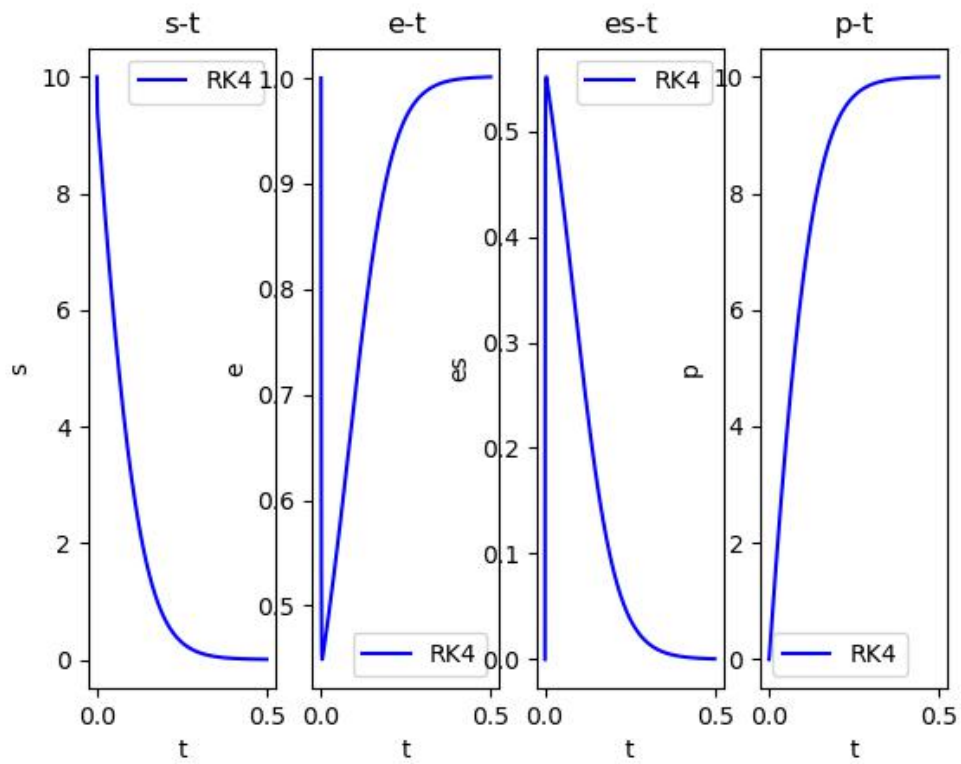
```
101. plt.title('v-t')
```

```
102. x = s[pt==np.max(pt)]
```

```
103. y = np.max(pt)
```

```
104. plt.plot(x,y,'r',marker='*')
```

```
105. plt.show()
```



The reason why there is a sudden drop to 0 later in the curve is, I think, to consider that the reaction starts with the maximum concentration, but the production rate increases from 0